Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID	:	2Q2E
Title	:	Crystal structure of the topoisomerase VI holoenzyme from Methanosarcina mazei
Authors	:	Corbett, K.D.; Benedetti, P.; Berger, J.M.
Deposited on	:	2007-05-28
Resolution	:	4.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

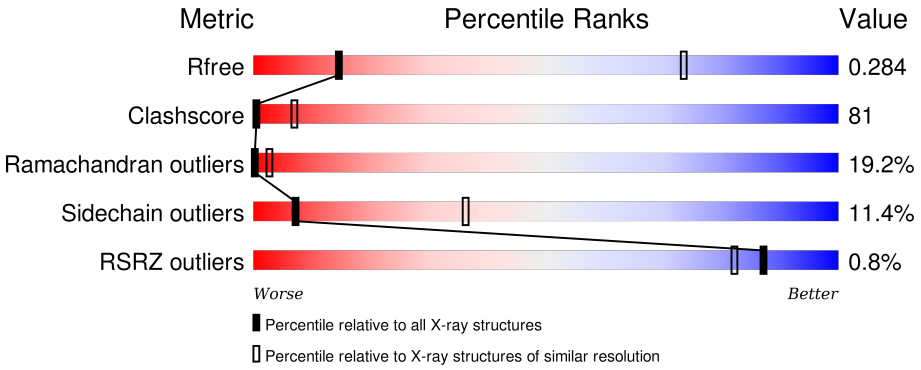
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	369	% 17% 51% 16% • 15%
2	B	621	19% 55% 18% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7039 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 Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2532	1610	423	490	9	0	0	0

- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

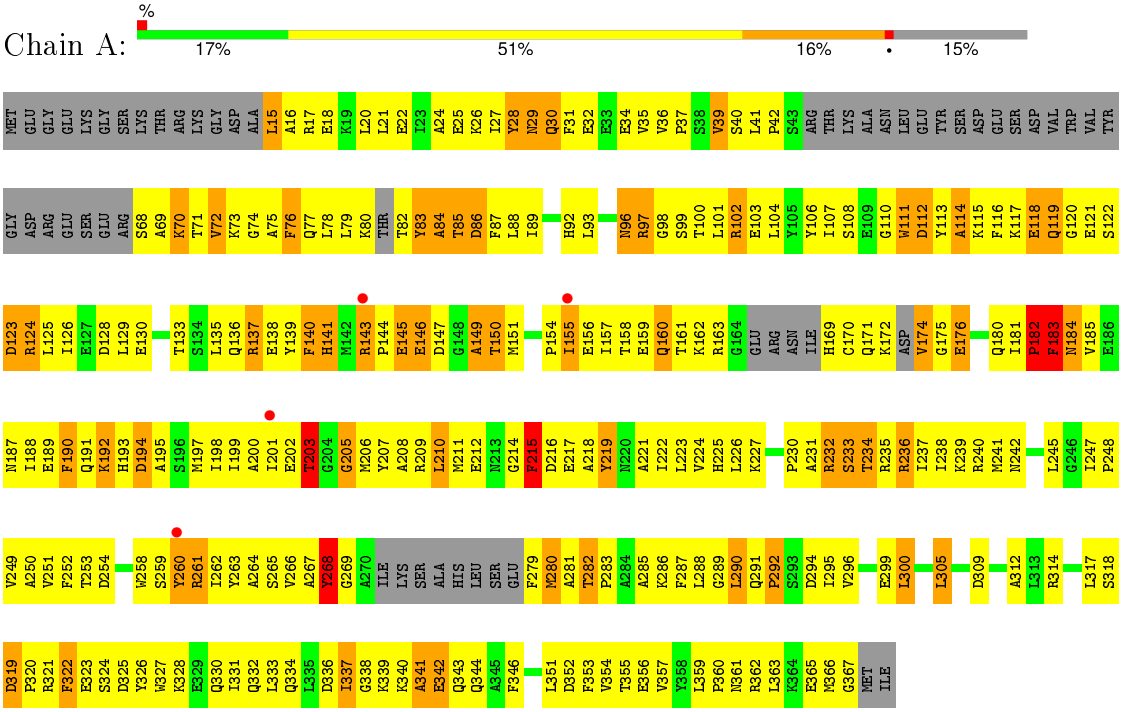
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	582	4507	2878	768	843	18	0	0	1

3 Residue-property plots (i)

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

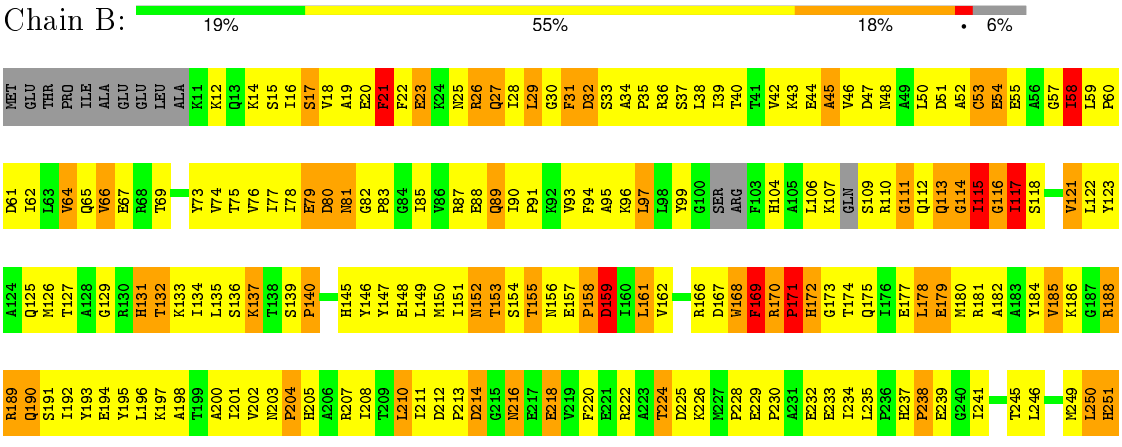
- Molecule 1: Type II DNA topoisomerase VI subunit A

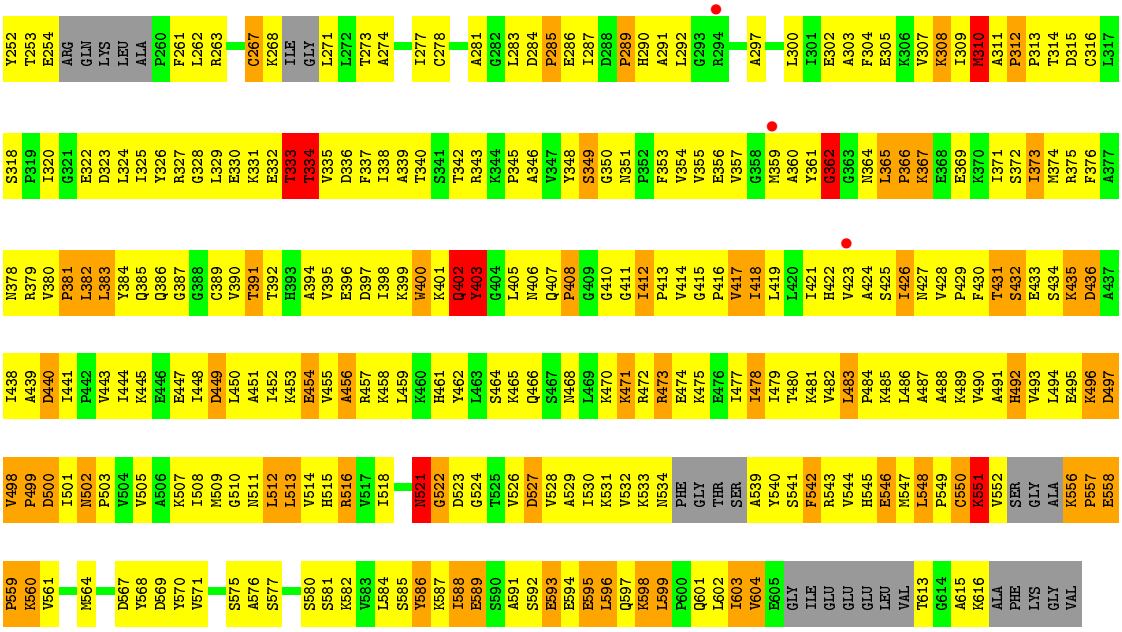
Chain A:



- Molecule 2: Type 2 DNA topoisomerase 6 subunit B

Chain B:




Y252 T253 E254 ARG GLN LYS LEU ALA P260 F261 L262 R263 C267 K268 ILE GLY L271 L272 T273 A274 I277 C278 A281 G282 L283 D284 P285 E286 I287 D288 P289 H290 A291 L292 G293 R294 A297 L300 I301 E302 A303 F304 E305 K306 V307 K308 I309 M310 A311 P312 P313 T314 D315 C316 L317
S318 P319 I320 G321 E322 D323 L324 I325 Y326 R327 G328 L329 E330 K331 E332 T333 T334 V335 D336 F337 I338 A339 T340 S341 T342 R343 K344 P345 A346 V347 Y348 S349 G350 N351 P352 F353 V354 V355 E356 V357 G358 M359 A360 Y361 G362 G363 N364 L365 P366 K367 E368 E369 K370 I371 S372 I373 M374 R375 F376 A377
N378 R379 V380 P381 L382 L383 Y384 Q385 Q386 G387 G388 C389 V390 T391 T392 H393 A394 V395 E396 D397 I398 K399 W400 K401 Q402 Y403 G404 L405 N406 Q407 P408 G409 G410 G411 I412 P413 V414 G415 P416 V417 I418 L419 L420 I421 H422 V423 A424 S425 I426 N427 V428 P429 F430 T431 S432 E433 S434 K435 D436 A437
I438 A439 D440 I441 P442 V443 I444 K445 E446 E447 I448 D449 L450 A451 I452 K453 E454 V455 A456 R457 K458 L459 K460 H461 Y462 L463 S464 K465 Q466 S467 N468 L469 K470 K471 R472 R473 E474 K475 E476 I477 I478 I479 T480 K481 V482 L483 P484 K485 L486 A487 A488 K489 V490 A491 H492 V493 L494 E495 K496 D497
V498 P499 D500 I501 N502 P503 V504 V505 A506 K507 I508 M509 G510 N511 L512 L513 V514 H515 R516 V517 I518 N521 G522 D523 G524 T525 V526 D527 V528 A529 I530 K531 V532 K533 N534 PHE GLY THR SER A539 Y540 S541 F542 R543 V544 H545 E546 M547 L548 P549 C550 K551 V552 SER GLY ALA K556 P557 E558
P559 K560 V561 M564 D567 Y568 D569 Y570 V571 S575 A576 S577 S580 S581 K582 V583 L584 S585 Y586 K587 I588 E589 S590 A591 S592 E593 E594 E595 L596 Q597 K598 L599 P600 Q601 L602 I603 V604 E605 GLY ILE GLU GLU GLU LEU VAL T613 G614 A615 K616 ALA PHE LYS GLY VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	227.81Å 227.81Å 208.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 92.23 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-4.00) 94.1 (92.23-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.306 , 0.349 0.296 , 0.284	Depositor DCC
R_{free} test set	1294 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	153.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 211.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 25919 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å^2)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/2579	0.71	0/3471
2	B	0.51	1/4591 (0.0%)	0.83	5/6215 (0.1%)
All	All	0.47	1/7170 (0.0%)	0.79	5/9686 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	CYS	CB-SG	-6.66	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	57	GLY	N-CA-C	5.88	127.79	113.10
2	B	408	PRO	N-CA-CB	5.82	110.29	103.30
2	B	522	GLY	N-CA-C	-5.75	98.72	113.10
2	B	58	ILE	N-CA-C	5.66	126.29	111.00
2	B	362	GLY	N-CA-C	5.42	126.64	113.10

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	2532	0	2476	393	0
2	B	4507	0	4565	779	0
All	All	7039	0	7041	1140	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 81.

All (1140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:LEU:H	2:B:599:LEU:HD23	1.09	1.13
2:B:516:ARG:HH12	2:B:597:GLN:HB2	0.93	1.09
2:B:371:ILE:HG22	2:B:414:VAL:HG12	1.13	1.09
2:B:66:VAL:HG23	2:B:213:PRO:HD3	1.35	1.08
2:B:222:ARG:HH21	2:B:332:GLU:HB2	1.12	1.06
2:B:238:PRO:HA	2:B:241:ILE:HD12	1.35	1.05
1:A:31:PHE:HB2	2:B:489:LYS:HD3	1.39	1.05
1:A:15:LEU:HD12	1:A:96:ASN:HA	1.38	1.05
2:B:137:LYS:HG3	2:B:171:PRO:HA	1.34	1.05
1:A:87:PHE:HA	2:B:492:HIS:NE2	1.73	1.03
2:B:201:ILE:HD11	2:B:329:LEU:HG	1.38	1.03
2:B:77:ILE:C	2:B:78:ILE:HD12	1.78	1.01
2:B:365:LEU:HB3	2:B:366:PRO:HD2	1.41	1.01
2:B:516:ARG:NH1	2:B:597:GLN:HB2	1.75	0.99
2:B:588:ILE:HG12	2:B:589:GLU:H	1.27	0.99
2:B:497:ASP:O	2:B:499:PRO:HD3	1.62	0.99
1:A:305:LEU:HD12	1:A:305:LEU:H	1.23	0.98
2:B:168:TRP:CE3	2:B:169:PHE:HA	1.97	0.97
2:B:190:GLN:HG2	2:B:383:LEU:HD21	1.45	0.97
2:B:222:ARG:NH2	2:B:332:GLU:HB2	1.80	0.97
2:B:232:GLU:CD	2:B:316:CYS:HA	1.84	0.96
2:B:359:MET:HE1	2:B:455:VAL:HG23	1.47	0.96
1:A:83:TYR:CD1	2:B:488:ALA:HB1	2.01	0.95
2:B:246:LEU:HD23	2:B:297:ALA:HB1	1.48	0.95
2:B:307:VAL:HG22	2:B:309:ILE:HD11	1.48	0.94
2:B:335:VAL:HG22	2:B:336:ASP:H	1.33	0.94
2:B:335:VAL:HG11	2:B:338:ILE:HD11	1.50	0.93
2:B:114:GLY:O	2:B:116:GLY:N	2.01	0.93
2:B:390:VAL:HG23	2:B:438:ILE:O	1.70	0.92
1:A:324:SER:HB3	1:A:327:TRP:HD1	1.34	0.92
1:A:203:THR:OG1	1:A:206:MET:HB3	1.68	0.92
2:B:210:LEU:HD12	2:B:211:ILE:N	1.85	0.91
1:A:253:THR:HB	1:A:259:SER:HB3	1.54	0.89
1:A:20:LEU:HD12	1:A:21:LEU:N	1.88	0.89
1:A:31:PHE:HB2	2:B:489:LYS:CD	2.03	0.89
1:A:239:LYS:NZ	1:A:279:PHE:HA	1.88	0.89
2:B:411:GLY:O	2:B:412:ILE:HG13	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HD11	1:A:207:TYR:HD1	1.37	0.88
1:A:28:TYR:HE1	2:B:489:LYS:HG2	1.38	0.87
2:B:552:VAL:HB	2:B:587:LYS:HB2	1.56	0.87
2:B:58:ILE:HG22	2:B:59:LEU:H	1.40	0.87
2:B:64:VAL:HG22	2:B:78:ILE:HG13	1.55	0.87
1:A:156:GLU:O	1:A:157:ILE:HG13	1.73	0.87
1:A:206:MET:H	1:A:344:GLN:HE21	1.23	0.87
2:B:546:GLU:HG3	2:B:548:LEU:HD11	1.57	0.86
2:B:61:ASP:HB2	2:B:207:ARG:HH11	1.38	0.86
2:B:367:LYS:HA	2:B:367:LYS:HE2	1.55	0.86
2:B:507:LYS:HG3	2:B:533:LYS:NZ	1.89	0.85
1:A:239:LYS:HD3	1:A:279:PHE:HD2	1.40	0.85
2:B:381:PRO:O	2:B:382:LEU:HB2	1.75	0.85
2:B:65:GLN:HG3	2:B:211:ILE:HG13	1.59	0.85
2:B:125:GLN:HE22	2:B:151:ILE:HB	1.42	0.85
1:A:185:VAL:HG21	1:A:236:ARG:HB3	1.56	0.84
2:B:490:VAL:C	2:B:492:HIS:H	1.79	0.84
1:A:28:TYR:CE1	2:B:489:LYS:HG2	2.13	0.83
1:A:69:ALA:HB2	1:A:78:LEU:HD11	1.60	0.83
2:B:569:ASP:OD2	2:B:571:VAL:HG23	1.78	0.83
1:A:188:ILE:HG12	1:A:240:ARG:NH2	1.93	0.83
1:A:188:ILE:HG21	1:A:240:ARG:CZ	2.08	0.82
2:B:335:VAL:HG22	2:B:336:ASP:N	1.94	0.82
2:B:497:ASP:CG	2:B:498:VAL:H	1.81	0.82
2:B:241:ILE:HG23	2:B:245:THR:HG21	1.60	0.82
2:B:96:LYS:HE2	2:B:114:GLY:HA3	1.60	0.82
1:A:197:MET:O	1:A:221:ALA:HA	1.79	0.82
2:B:371:ILE:CG2	2:B:414:VAL:HG12	2.04	0.81
1:A:338:GLY:O	1:A:339:LYS:HG3	1.80	0.81
1:A:252:PHE:HD1	1:A:289:GLY:HA2	1.41	0.81
2:B:401:LYS:HZ3	2:B:406:ASN:HD21	1.26	0.81
2:B:127:THR:CG2	2:B:181:ARG:HB3	2.09	0.81
2:B:168:TRP:O	2:B:169:PHE:HB2	1.80	0.81
1:A:324:SER:HB3	1:A:327:TRP:CD1	2.16	0.81
2:B:137:LYS:CG	2:B:172:HIS:H	1.95	0.81
1:A:31:PHE:CB	2:B:489:LYS:HD3	2.11	0.80
2:B:453:LYS:HE2	2:B:457:ARG:NH2	1.95	0.80
1:A:342:GLU:HG3	1:A:343:GLN:H	1.47	0.80
1:A:252:PHE:CD1	1:A:289:GLY:HA2	2.15	0.80
1:A:188:ILE:HG21	1:A:240:ARG:NE	1.95	0.80
1:A:237:ILE:HG22	1:A:241:MET:HE2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HB2	1:A:140:PHE:CE1	2.16	0.80
1:A:69:ALA:CB	1:A:78:LEU:HD11	2.11	0.80
1:A:202:GLU:O	1:A:203:THR:HG23	1.82	0.80
1:A:161:THR:HG23	1:A:162:LYS:HG3	1.64	0.80
1:A:101:LEU:HD22	1:A:122:SER:HB3	1.64	0.80
2:B:107:LYS:HZ2	2:B:378:ASN:CG	1.84	0.80
1:A:198:ILE:HB	1:A:249:VAL:HG22	1.64	0.80
2:B:501:ILE:O	2:B:505:VAL:HG23	1.82	0.79
2:B:557:PRO:HG3	2:B:584:LEU:HA	1.63	0.79
1:A:169:HIS:O	1:A:174:VAL:HG13	1.82	0.79
2:B:27:GLN:HG2	2:B:32:ASP:HB2	1.62	0.79
2:B:595:GLU:O	2:B:596:LEU:HG	1.82	0.79
2:B:599:LEU:HD23	2:B:599:LEU:N	1.94	0.78
1:A:239:LYS:HZ3	1:A:279:PHE:HA	1.46	0.78
2:B:375:ARG:NH1	2:B:382:LEU:HD23	1.99	0.78
1:A:70:LYS:HG2	1:A:71:THR:HG23	1.64	0.78
1:A:88:LEU:O	1:A:92:HIS:HB2	1.83	0.78
1:A:363:LEU:HD23	1:A:363:LEU:O	1.83	0.78
2:B:65:GLN:O	2:B:66:VAL:HG13	1.83	0.78
2:B:365:LEU:HB3	2:B:366:PRO:CD	2.12	0.78
2:B:127:THR:HG21	2:B:181:ARG:HB3	1.64	0.77
2:B:597:GLN:O	2:B:598:LYS:HB3	1.82	0.77
1:A:31:PHE:CE1	1:A:32:GLU:HG3	2.20	0.77
1:A:133:THR:HG1	1:A:140:PHE:HZ	1.29	0.77
2:B:80:ASP:OD1	2:B:174:THR:HG23	1.85	0.77
1:A:133:THR:O	1:A:135:LEU:HG	1.84	0.77
2:B:375:ARG:HH11	2:B:375:ARG:HG3	1.49	0.77
1:A:242:ASN:OD1	1:A:282:THR:HG23	1.84	0.76
1:A:290:LEU:HD21	1:A:341:ALA:HB1	1.68	0.76
1:A:200:ALA:HB3	1:A:251:VAL:HA	1.68	0.76
2:B:465:LYS:O	2:B:468:ASN:HB3	1.86	0.76
2:B:335:VAL:HG11	2:B:338:ILE:CD1	2.15	0.75
1:A:154:PRO:HG2	1:A:195:ALA:HB2	1.69	0.75
2:B:60:PRO:HA	2:B:81:ASN:ND2	2.00	0.75
2:B:73:TYR:CE1	2:B:181:ARG:HB2	2.22	0.75
2:B:145:HIS:HB3	2:B:147:TYR:CE1	2.22	0.75
1:A:20:LEU:HB2	1:A:135:LEU:HD13	1.68	0.75
2:B:551:LYS:HG2	2:B:552:VAL:N	2.01	0.75
2:B:77:ILE:N	2:B:77:ILE:HD12	2.02	0.75
2:B:353:PHE:HA	2:B:424:ALA:O	1.86	0.75
2:B:106:LEU:HB2	2:B:232:GLU:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:HG3	2:B:172:HIS:H	1.52	0.74
1:A:31:PHE:O	1:A:35:VAL:HG23	1.86	0.74
2:B:107:LYS:HZ2	2:B:378:ASN:ND2	1.86	0.74
1:A:328:LYS:O	1:A:332:GLN:HG3	1.88	0.74
2:B:184:TYR:HE1	2:B:192:ILE:HG12	1.51	0.74
1:A:15:LEU:HD13	1:A:93:LEU:O	1.87	0.74
2:B:171:PRO:O	2:B:172:HIS:HB2	1.88	0.74
2:B:561:VAL:HG22	2:B:570:TYR:CD1	2.22	0.74
2:B:188:ARG:O	2:B:190:GLN:N	2.21	0.74
2:B:210:LEU:HD12	2:B:210:LEU:C	2.08	0.73
2:B:453:LYS:HE2	2:B:457:ARG:HH21	1.53	0.73
2:B:125:GLN:O	2:B:129:GLY:HA2	1.88	0.73
2:B:37:SER:HB2	2:B:182:ALA:HB1	1.70	0.73
2:B:551:LYS:HE3	2:B:552:VAL:C	2.09	0.73
2:B:507:LYS:HG3	2:B:533:LYS:HZ2	1.51	0.73
1:A:35:VAL:HG11	2:B:486:LEU:HD13	1.70	0.73
2:B:473:ARG:HG3	2:B:473:ARG:HH11	1.53	0.73
2:B:390:VAL:HG22	2:B:440:ASP:HA	1.70	0.73
1:A:72:VAL:H	2:B:478:ILE:HD11	1.53	0.73
2:B:222:ARG:HH21	2:B:332:GLU:CB	1.97	0.73
1:A:225:HIS:O	1:A:226:LEU:HD23	1.89	0.73
2:B:532:VAL:HG22	2:B:533:LYS:N	2.04	0.73
2:B:528:VAL:HG12	2:B:584:LEU:HD12	1.71	0.73
2:B:599:LEU:H	2:B:599:LEU:CD2	1.91	0.72
2:B:411:GLY:C	2:B:412:ILE:HG13	2.08	0.72
2:B:322:GLU:O	2:B:340:THR:HG21	1.89	0.72
2:B:133:LYS:HB3	2:B:177:GLU:HB3	1.72	0.72
1:A:264:ALA:HA	1:A:267:ALA:HB3	1.70	0.72
2:B:202:VAL:C	2:B:204:PRO:HD3	2.09	0.72
2:B:232:GLU:OE1	2:B:316:CYS:HA	1.87	0.72
2:B:74:VAL:O	2:B:179:GLU:HA	1.89	0.72
1:A:135:LEU:HB2	1:A:140:PHE:HE1	1.54	0.72
2:B:76:VAL:HG12	2:B:78:ILE:HD11	1.70	0.72
1:A:356:GLU:O	1:A:360:PRO:HG3	1.90	0.71
2:B:588:ILE:HG12	2:B:589:GLU:N	2.02	0.71
2:B:222:ARG:HH12	2:B:331:LYS:HB2	1.54	0.71
2:B:401:LYS:NZ	2:B:406:ASN:HD21	1.88	0.71
2:B:237:HIS:CD2	2:B:312:PRO:HG3	2.26	0.71
2:B:490:VAL:O	2:B:492:HIS:N	2.22	0.71
1:A:342:GLU:HG3	1:A:343:GLN:N	2.05	0.71
2:B:149:LEU:HD12	2:B:150:MET:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:C	1:A:31:PHE:H	1.92	0.71
1:A:279:PHE:O	1:A:280:MET:HG3	1.90	0.70
2:B:561:VAL:HG22	2:B:570:TYR:HD1	1.54	0.70
2:B:335:VAL:HG21	2:B:360:ALA:HB1	1.73	0.70
1:A:78:LEU:HB3	2:B:485:LYS:NZ	2.07	0.70
2:B:184:TYR:CE1	2:B:192:ILE:HG21	2.27	0.70
2:B:114:GLY:C	2:B:116:GLY:H	1.94	0.70
2:B:78:ILE:N	2:B:78:ILE:HD12	2.06	0.70
1:A:234:THR:O	1:A:237:ILE:HB	1.92	0.70
2:B:238:PRO:HG2	2:B:239:GLU:OE1	1.90	0.69
2:B:241:ILE:HG23	2:B:245:THR:CG2	2.22	0.69
2:B:348:TYR:O	2:B:350:GLY:N	2.25	0.69
2:B:137:LYS:HE3	2:B:173:GLY:H	1.55	0.69
2:B:112:GLN:HB2	2:B:435:LYS:HD3	1.74	0.69
2:B:113:GLN:O	2:B:115:ILE:HG13	1.92	0.69
2:B:508:ILE:CG2	2:B:509:MET:N	2.55	0.69
1:A:235:ARG:HD3	1:A:265:SER:O	1.92	0.69
2:B:235:LEU:HD12	2:B:267:CYS:HB3	1.74	0.69
1:A:154:PRO:O	1:A:155:ILE:HG23	1.92	0.69
2:B:65:GLN:HG2	2:B:66:VAL:H	1.56	0.69
2:B:237:HIS:CG	2:B:312:PRO:HG3	2.27	0.69
2:B:232:GLU:OE2	2:B:316:CYS:HA	1.91	0.69
1:A:20:LEU:HB2	1:A:135:LEU:CD1	2.22	0.69
1:A:15:LEU:CD1	1:A:96:ASN:HA	2.18	0.69
2:B:170:ARG:HG2	2:B:170:ARG:HH11	1.57	0.69
2:B:90:ILE:HG22	2:B:91:PRO:N	2.08	0.69
2:B:557:PRO:HD3	2:B:585:SER:H	1.57	0.69
2:B:396:GLU:HG2	2:B:412:ILE:HG23	1.75	0.69
2:B:212:ASP:HB2	2:B:213:PRO:HD2	1.75	0.69
2:B:360:ALA:HB3	2:B:418:ILE:CG2	2.22	0.69
2:B:400:TRP:HZ3	2:B:408:PRO:HA	1.58	0.68
2:B:139:SER:HB2	2:B:140:PRO:HD2	1.74	0.68
2:B:334:THR:HB	2:B:364:ASN:HB2	1.75	0.68
1:A:253:THR:CB	1:A:259:SER:HB3	2.24	0.68
2:B:107:LYS:HG3	2:B:378:ASN:HD21	1.59	0.68
1:A:157:ILE:HG22	1:A:158:THR:N	2.08	0.68
2:B:355:VAL:HG22	2:B:423:VAL:HG12	1.76	0.68
1:A:236:ARG:HG3	1:A:280:MET:HG3	1.74	0.68
2:B:38:LEU:HD13	2:B:184:TYR:HB2	1.76	0.68
1:A:79:LEU:O	1:A:79:LEU:HD23	1.93	0.68
2:B:345:PRO:HA	2:B:354:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLY:O	1:A:215:PHE:HB2	1.92	0.68
2:B:531:LYS:HE2	2:B:581:SER:HB2	1.76	0.68
2:B:324:LEU:H	2:B:324:LEU:HD12	1.60	0.67
2:B:66:VAL:O	2:B:213:PRO:HD3	1.94	0.67
1:A:27:ILE:HD11	1:A:133:THR:HG21	1.76	0.67
2:B:425:SER:OG	2:B:428:VAL:HG22	1.94	0.67
1:A:117:LYS:NZ	1:A:117:LYS:HB2	2.10	0.67
1:A:239:LYS:HD3	1:A:279:PHE:CD2	2.27	0.67
2:B:137:LYS:HE3	2:B:173:GLY:CA	2.25	0.67
2:B:516:ARG:HH12	2:B:597:GLN:CB	1.89	0.67
2:B:38:LEU:HA	2:B:180:MET:CE	2.25	0.67
2:B:335:VAL:CG2	2:B:336:ASP:H	2.07	0.67
2:B:531:LYS:CD	2:B:581:SER:HB2	2.25	0.67
2:B:137:LYS:HE3	2:B:173:GLY:N	2.10	0.67
2:B:320:ILE:CD1	2:B:379:ARG:HH11	2.08	0.67
2:B:343:ARG:HH11	2:B:343:ARG:HG3	1.59	0.67
2:B:342:THR:HG23	2:B:356:GLU:HG2	1.77	0.67
2:B:518:ILE:HG22	2:B:526:VAL:HG13	1.77	0.67
1:A:112:ASP:O	1:A:114:ALA:N	2.28	0.66
1:A:39:VAL:HG12	1:A:40:SER:H	1.61	0.66
2:B:366:PRO:O	2:B:416:PRO:HG3	1.95	0.66
1:A:201:ILE:HD11	1:A:207:TYR:CD1	2.26	0.66
2:B:576:ALA:HB1	2:B:580:SER:HB3	1.78	0.66
2:B:36:ARG:HA	2:B:39:ILE:HG22	1.77	0.66
1:A:181:ILE:O	1:A:181:ILE:HG13	1.94	0.66
2:B:66:VAL:HG12	2:B:76:VAL:HG22	1.75	0.66
2:B:48:ASN:HD21	2:B:117:ILE:HG12	1.61	0.66
1:A:230:PRO:HD3	1:A:262:ILE:HG23	1.77	0.66
2:B:27:GLN:CG	2:B:32:ASP:HB2	2.26	0.66
1:A:282:THR:O	1:A:282:THR:HG22	1.94	0.65
2:B:66:VAL:HA	2:B:75:THR:O	1.96	0.65
1:A:35:VAL:HG21	2:B:486:LEU:HD22	1.77	0.65
2:B:514:VAL:HG12	2:B:530:ILE:HG12	1.77	0.65
2:B:192:ILE:HG23	2:B:193:TYR:H	1.61	0.65
2:B:307:VAL:HG13	2:B:307:VAL:O	1.96	0.65
2:B:205:HIS:CD2	2:B:228:PRO:HD3	2.32	0.65
2:B:290:HIS:CG	2:B:291:ALA:N	2.64	0.65
1:A:326:TYR:O	1:A:330:GLN:HG2	1.96	0.65
2:B:190:GLN:CG	2:B:383:LEU:HD11	2.27	0.65
2:B:246:LEU:HD23	2:B:297:ALA:CB	2.26	0.65
2:B:96:LYS:C	2:B:97:LEU:HD23	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:O	1:A:281:ALA:HA	1.97	0.65
1:A:282:THR:HG22	1:A:285:ALA:HB2	1.79	0.65
2:B:490:VAL:C	2:B:492:HIS:N	2.50	0.65
1:A:233:SER:O	1:A:237:ILE:HG12	1.97	0.65
2:B:586:TYR:C	2:B:587:LYS:HD3	2.17	0.65
2:B:66:VAL:CG1	2:B:76:VAL:HG13	2.27	0.65
2:B:112:GLN:OE1	2:B:112:GLN:HA	1.96	0.65
2:B:284:ASP:HB2	2:B:287:ILE:HG23	1.78	0.65
2:B:399:LYS:HG2	2:B:403:TYR:CD1	2.33	0.64
1:A:83:TYR:O	1:A:85:THR:N	2.29	0.64
2:B:94:PHE:CD1	2:B:134:ILE:HD11	2.32	0.64
2:B:60:PRO:HA	2:B:81:ASN:HD22	1.60	0.64
1:A:206:MET:N	1:A:344:GLN:HE21	1.94	0.64
1:A:154:PRO:CG	1:A:195:ALA:HB2	2.25	0.64
1:A:159:GLU:O	1:A:160:GLN:HB2	1.97	0.64
2:B:576:ALA:HB2	2:B:582:LYS:HE3	1.80	0.64
1:A:133:THR:OG1	1:A:140:PHE:HZ	1.79	0.64
1:A:157:ILE:HG12	1:A:190:PHE:HA	1.79	0.64
2:B:371:ILE:HG21	2:B:413:PRO:O	1.97	0.64
2:B:523:ASP:O	2:B:588:ILE:HD12	1.97	0.64
2:B:229:GLU:HG3	2:B:230:PRO:HD2	1.79	0.64
1:A:31:PHE:CG	1:A:32:GLU:N	2.66	0.64
2:B:375:ARG:HD2	2:B:382:LEU:HD23	1.79	0.64
1:A:200:ALA:HB3	1:A:250:ALA:O	1.98	0.64
1:A:181:ILE:CD1	1:A:237:ILE:HG13	2.28	0.64
1:A:268:TYR:HB2	1:A:322:PHE:HE2	1.62	0.64
2:B:495:GLU:O	2:B:497:ASP:N	2.31	0.64
2:B:189:ARG:O	2:B:190:GLN:CB	2.46	0.64
2:B:412:ILE:HD12	2:B:412:ILE:O	1.98	0.64
2:B:309:ILE:HG22	2:B:310:MET:N	2.13	0.64
2:B:151:ILE:O	2:B:152:ASN:C	2.35	0.64
2:B:400:TRP:HZ2	2:B:411:GLY:N	1.96	0.64
2:B:151:ILE:O	2:B:151:ILE:HG22	1.97	0.64
1:A:104:LEU:HD23	1:A:122:SER:OG	1.98	0.64
2:B:531:LYS:CE	2:B:581:SER:HB2	2.28	0.64
2:B:367:LYS:O	2:B:416:PRO:HG3	1.98	0.63
2:B:373:ILE:HG12	2:B:373:ILE:O	1.99	0.63
2:B:325:ILE:O	2:B:329:LEU:HD12	1.98	0.63
1:A:137:ARG:HD3	1:A:232:ARG:HE	1.63	0.63
2:B:50:LEU:HB3	2:B:54:GLU:OE2	1.98	0.63
2:B:36:ARG:HG3	2:B:384:TYR:OH	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:PHE:O	2:B:422:HIS:HA	1.99	0.63
2:B:309:ILE:HG22	2:B:310:MET:H	1.61	0.63
1:A:155:ILE:O	1:A:170:CYS:HB3	1.99	0.63
2:B:34:ALA:N	2:B:35:PRO:HD2	2.14	0.63
2:B:601:GLN:N	2:B:601:GLN:OE1	2.31	0.63
1:A:28:TYR:O	1:A:31:PHE:N	2.31	0.63
1:A:24:ALA:O	1:A:27:ILE:HD12	1.98	0.63
2:B:233:GLU:HG2	2:B:234:ILE:N	2.14	0.63
2:B:290:HIS:CG	2:B:291:ALA:H	2.16	0.63
2:B:107:LYS:NZ	2:B:378:ASN:ND2	2.46	0.63
2:B:135:LEU:HD23	2:B:169:PHE:CE2	2.34	0.63
2:B:127:THR:HG22	2:B:181:ARG:HB3	1.81	0.63
1:A:149:ALA:CA	1:A:180:GLN:HG3	2.29	0.63
2:B:527:ASP:OD2	2:B:585:SER:HB3	1.99	0.63
1:A:203:THR:C	1:A:205:GLY:H	2.00	0.63
2:B:507:LYS:HE3	2:B:533:LYS:HZ3	1.64	0.63
2:B:302:GLU:HA	2:B:305:GLU:CG	2.29	0.63
2:B:399:LYS:O	2:B:400:TRP:CD1	2.52	0.62
1:A:346:PHE:HD1	1:A:354:VAL:HG22	1.64	0.62
2:B:543:ARG:O	2:B:601:GLN:HB3	1.99	0.62
2:B:239:GLU:O	2:B:350:GLY:HA3	1.99	0.62
2:B:549:PRO:HG3	2:B:567:ASP:OD1	2.00	0.62
2:B:168:TRP:CE3	2:B:169:PHE:CA	2.78	0.62
1:A:84:ALA:HB1	1:A:111:TRP:CE2	2.34	0.62
2:B:399:LYS:O	2:B:400:TRP:HB2	2.00	0.62
2:B:64:VAL:CG2	2:B:78:ILE:HG13	2.27	0.62
2:B:58:ILE:HG22	2:B:59:LEU:N	2.11	0.62
2:B:548:LEU:HD12	2:B:548:LEU:N	2.15	0.62
1:A:31:PHE:CD1	1:A:32:GLU:N	2.67	0.62
1:A:98:GLY:HA3	1:A:141:HIS:CE1	2.35	0.62
2:B:233:GLU:O	2:B:234:ILE:HG23	1.99	0.62
2:B:400:TRP:HH2	2:B:410:GLY:H	1.42	0.62
2:B:66:VAL:HG13	2:B:76:VAL:HG13	1.82	0.62
2:B:508:ILE:HG22	2:B:509:MET:H	1.64	0.62
2:B:125:GLN:NE2	2:B:151:ILE:HB	2.14	0.62
1:A:198:ILE:O	1:A:199:ILE:HD13	1.99	0.62
2:B:196:LEU:O	2:B:200:ALA:N	2.25	0.62
1:A:108:SER:HA	1:A:111:TRP:NE1	2.15	0.61
2:B:114:GLY:C	2:B:116:GLY:N	2.51	0.61
2:B:400:TRP:CZ3	2:B:407:GLN:O	2.53	0.61
2:B:238:PRO:HA	2:B:241:ILE:CD1	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLY:O	2:B:118:SER:N	2.33	0.61
1:A:150:THR:CB	1:A:225:HIS:HB3	2.29	0.61
2:B:507:LYS:HG3	2:B:533:LYS:HZ3	1.63	0.61
2:B:512:LEU:HD11	2:B:542:PHE:CE2	2.35	0.61
2:B:417:VAL:HG12	2:B:418:ILE:H	1.63	0.61
1:A:205:GLY:HA3	1:A:344:GLN:HE22	1.66	0.61
1:A:157:ILE:HG23	1:A:189:GLU:HB3	1.82	0.61
2:B:591:ALA:O	2:B:593:GLU:HG2	1.99	0.61
1:A:208:ALA:O	1:A:211:MET:HB3	2.01	0.61
2:B:222:ARG:HH22	2:B:332:GLU:N	1.98	0.61
1:A:28:TYR:O	1:A:31:PHE:HB3	2.00	0.61
2:B:36:ARG:NE	2:B:384:TYR:CE2	2.68	0.61
2:B:61:ASP:HB2	2:B:207:ARG:NH1	2.12	0.61
2:B:598:LYS:HE2	2:B:613:THR:CB	2.31	0.61
2:B:307:VAL:HG22	2:B:309:ILE:CD1	2.28	0.61
1:A:80:LYS:HD2	1:A:116:PHE:HE1	1.66	0.61
1:A:124:ARG:O	1:A:128:ASP:N	2.33	0.61
1:A:183:PHE:O	1:A:184:ASN:HB2	2.01	0.61
2:B:66:VAL:HG23	2:B:213:PRO:CD	2.21	0.61
2:B:360:ALA:O	2:B:418:ILE:HG22	2.00	0.61
2:B:96:LYS:O	2:B:97:LEU:HD23	2.00	0.61
1:A:157:ILE:CG2	1:A:158:THR:N	2.64	0.61
2:B:137:LYS:HG2	2:B:172:HIS:H	1.66	0.61
2:B:478:ILE:O	2:B:478:ILE:HG22	2.01	0.61
2:B:482:VAL:HG11	2:B:505:VAL:HG22	1.82	0.61
2:B:545:HIS:CG	2:B:571:VAL:HG22	2.35	0.61
2:B:399:LYS:HG2	2:B:403:TYR:CG	2.36	0.60
2:B:169:PHE:HD1	2:B:169:PHE:O	1.84	0.60
2:B:73:TYR:HA	2:B:181:ARG:HA	1.83	0.60
1:A:28:TYR:O	1:A:30:GLN:N	2.34	0.60
2:B:430:PHE:CD1	2:B:435:LYS:HA	2.36	0.60
1:A:28:TYR:C	1:A:31:PHE:HD2	2.05	0.60
2:B:250:LEU:O	2:B:252:TYR:N	2.33	0.60
1:A:287:PHE:CE1	1:A:289:GLY:HA3	2.36	0.60
1:A:351:LEU:HD12	1:A:351:LEU:N	2.15	0.60
2:B:241:ILE:HG23	2:B:245:THR:CB	2.31	0.60
2:B:399:LYS:O	2:B:400:TRP:CB	2.49	0.60
2:B:532:VAL:HG22	2:B:533:LYS:H	1.65	0.60
1:A:17:ARG:HH12	1:A:141:HIS:CB	2.14	0.60
2:B:125:GLN:HE22	2:B:151:ILE:CB	2.13	0.60
2:B:464:SER:O	2:B:468:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ARG:O	2:B:190:GLN:HB3	2.02	0.60
1:A:79:LEU:CD2	1:A:114:ALA:HB2	2.31	0.60
2:B:550:CYS:O	2:B:551:LYS:HB3	2.00	0.60
2:B:514:VAL:HG23	2:B:514:VAL:O	1.99	0.60
1:A:17:ARG:HD2	1:A:139:TYR:O	2.02	0.60
1:A:263:TYR:O	1:A:267:ALA:N	2.35	0.60
1:A:69:ALA:O	1:A:70:LYS:HB3	2.02	0.60
2:B:320:ILE:HD13	2:B:379:ARG:HH11	1.64	0.60
2:B:135:LEU:HD12	2:B:145:HIS:O	2.01	0.59
2:B:106:LEU:HD23	2:B:106:LEU:H	1.67	0.59
2:B:220:PHE:HD2	2:B:332:GLU:CD	2.05	0.59
2:B:497:ASP:CG	2:B:498:VAL:N	2.54	0.59
2:B:430:PHE:CZ	2:B:435:LYS:HG2	2.37	0.59
2:B:125:GLN:OE1	2:B:150:MET:HA	2.01	0.59
1:A:78:LEU:HB3	2:B:485:LYS:HZ2	1.65	0.59
2:B:75:THR:HG23	2:B:179:GLU:OE1	2.02	0.59
2:B:137:LYS:HE3	2:B:173:GLY:C	2.21	0.59
2:B:375:ARG:NH1	2:B:375:ARG:HG3	2.17	0.59
1:A:360:PRO:HG2	1:A:361:ASN:H	1.67	0.59
1:A:123:ASP:O	1:A:124:ARG:C	2.40	0.59
2:B:500:ASP:O	2:B:503:PRO:HD2	2.02	0.59
1:A:102:ARG:HD3	1:A:119:GLN:NE2	2.17	0.59
2:B:507:LYS:HE3	2:B:533:LYS:NZ	2.18	0.59
2:B:33:SER:HB3	2:B:35:PRO:HD2	1.84	0.59
2:B:448:ILE:O	2:B:451:ALA:HB3	2.02	0.59
1:A:150:THR:OG1	1:A:225:HIS:HB3	2.03	0.59
2:B:192:ILE:HG23	2:B:193:TYR:N	2.17	0.59
1:A:206:MET:HG2	1:A:343:GLN:HE21	1.68	0.59
1:A:231:ALA:HA	1:A:235:ARG:NH2	2.18	0.59
2:B:263:ARG:HD2	2:B:271:LEU:HG	1.84	0.59
2:B:197:LYS:HA	2:B:220:PHE:CE2	2.37	0.59
2:B:53:CYS:O	2:B:55:GLU:N	2.35	0.59
1:A:69:ALA:HA	1:A:74:GLY:O	2.02	0.59
2:B:73:TYR:CD1	2:B:181:ARG:HB2	2.38	0.59
2:B:110:ARG:HG3	2:B:380:VAL:HG22	1.84	0.58
1:A:20:LEU:HD22	1:A:139:TYR:HB3	1.85	0.58
2:B:150:MET:HE3	2:B:152:ASN:HB2	1.84	0.58
2:B:531:LYS:HG2	2:B:581:SER:HA	1.86	0.58
1:A:201:ILE:HD12	1:A:207:TYR:HA	1.86	0.58
2:B:601:GLN:OE1	2:B:613:THR:O	2.21	0.58
1:A:21:LEU:O	1:A:25:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ILE:N	2:B:115:ILE:HD12	2.18	0.58
2:B:205:HIS:NE2	2:B:228:PRO:HD3	2.18	0.58
2:B:263:ARG:NH1	2:B:271:LEU:HD11	2.18	0.58
2:B:455:VAL:O	2:B:457:ARG:N	2.37	0.58
1:A:31:PHE:O	1:A:35:VAL:N	2.36	0.58
2:B:90:ILE:HG12	2:B:147:TYR:CD2	2.39	0.58
2:B:64:VAL:O	2:B:64:VAL:HG12	2.03	0.58
2:B:588:ILE:CG1	2:B:589:GLU:H	2.10	0.58
2:B:407:GLN:CB	2:B:414:VAL:H	2.17	0.58
1:A:31:PHE:HB2	2:B:489:LYS:NZ	2.19	0.58
1:A:230:PRO:CD	1:A:262:ILE:HG23	2.34	0.58
2:B:357:VAL:HG11	2:B:452:ILE:HA	1.85	0.57
2:B:239:GLU:OE1	2:B:239:GLU:N	2.35	0.57
1:A:156:GLU:HG2	1:A:157:ILE:N	2.18	0.57
1:A:87:PHE:HD1	2:B:492:HIS:CD2	2.22	0.57
1:A:17:ARG:HH12	1:A:141:HIS:CG	2.22	0.57
1:A:326:TYR:O	1:A:330:GLN:NE2	2.30	0.57
2:B:69:THR:HG21	2:B:75:THR:HG23	1.87	0.57
2:B:237:HIS:CG	2:B:238:PRO:HD2	2.39	0.57
1:A:35:VAL:CG1	2:B:486:LEU:HD13	2.34	0.57
1:A:28:TYR:CZ	2:B:489:LYS:HA	2.39	0.57
2:B:430:PHE:CE2	2:B:435:LYS:HG2	2.39	0.57
1:A:201:ILE:HG22	1:A:252:PHE:HB3	1.87	0.57
2:B:549:PRO:HB2	2:B:589:GLU:OE2	2.05	0.57
2:B:345:PRO:CA	2:B:354:VAL:HG12	2.35	0.57
2:B:514:VAL:HG12	2:B:530:ILE:CG1	2.34	0.57
1:A:21:LEU:HD23	1:A:21:LEU:O	2.05	0.57
1:A:237:ILE:HG22	1:A:241:MET:CE	2.32	0.57
1:A:118:GLU:C	1:A:120:GLY:H	2.07	0.57
2:B:213:PRO:O	2:B:214:ASP:OD1	2.23	0.57
2:B:374:MET:CE	2:B:418:ILE:HD11	2.35	0.57
1:A:191:GLN:O	1:A:192:LYS:HB2	2.03	0.57
1:A:112:ASP:C	1:A:114:ALA:N	2.56	0.57
1:A:206:MET:CE	1:A:354:VAL:HG11	2.35	0.57
1:A:79:LEU:HD22	1:A:114:ALA:HB2	1.87	0.57
2:B:38:LEU:HA	2:B:180:MET:HE3	1.86	0.57
2:B:211:ILE:O	2:B:211:ILE:HG13	2.05	0.57
1:A:102:ARG:HD3	1:A:119:GLN:HE22	1.68	0.57
2:B:384:TYR:HB2	2:B:436:ASP:OD1	2.05	0.57
2:B:455:VAL:C	2:B:457:ARG:N	2.58	0.57
1:A:232:ARG:O	1:A:233:SER:C	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ILE:HG22	2:B:452:ILE:HD11	1.87	0.56
2:B:80:ASP:O	2:B:81:ASN:CB	2.52	0.56
2:B:149:LEU:HD12	2:B:150:MET:N	2.19	0.56
1:A:121:GLU:O	1:A:122:SER:C	2.43	0.56
1:A:282:THR:N	1:A:283:PRO:CD	2.69	0.56
1:A:159:GLU:O	1:A:160:GLN:CB	2.54	0.56
2:B:253:THR:HG22	2:B:254:GLU:N	2.21	0.56
2:B:597:GLN:O	2:B:598:LYS:CB	2.50	0.56
2:B:401:LYS:NZ	2:B:406:ASN:ND2	2.53	0.56
1:A:18:GLU:C	1:A:20:LEU:H	2.09	0.56
2:B:135:LEU:HD23	2:B:169:PHE:HE2	1.70	0.56
2:B:473:ARG:NH1	2:B:473:ARG:HG3	2.20	0.56
2:B:557:PRO:CD	2:B:585:SER:H	2.19	0.56
2:B:278:CYS:HB2	2:B:285:PRO:HG3	1.87	0.56
2:B:188:ARG:HG3	2:B:189:ARG:H	1.70	0.56
2:B:320:ILE:HD13	2:B:379:ARG:NH1	2.21	0.56
2:B:400:TRP:CZ2	2:B:411:GLY:N	2.74	0.56
2:B:26:ARG:HH11	2:B:26:ARG:HG2	1.70	0.56
1:A:282:THR:H	1:A:283:PRO:CD	2.18	0.56
1:A:300:LEU:HD11	1:A:346:PHE:CE2	2.40	0.56
2:B:399:LYS:HA	2:B:399:LYS:HE3	1.88	0.56
2:B:77:ILE:O	2:B:78:ILE:HD12	2.05	0.56
1:A:203:THR:N	1:A:225:HIS:NE2	2.44	0.56
2:B:485:LYS:C	2:B:487:ALA:H	2.09	0.56
1:A:209:ARG:O	1:A:209:ARG:HG2	2.05	0.56
2:B:394:ALA:HA	2:B:445:LYS:HE3	1.86	0.56
2:B:21:PHE:HD1	2:B:21:PHE:O	1.88	0.56
1:A:162:LYS:NZ	1:A:182:PRO:HG2	2.20	0.56
1:A:249:VAL:O	1:A:285:ALA:HB1	2.06	0.56
1:A:290:LEU:HD21	1:A:341:ALA:CB	2.35	0.56
2:B:148:GLU:HB2	2:B:162:VAL:HG23	1.85	0.56
2:B:375:ARG:CD	2:B:382:LEU:HD23	2.36	0.56
2:B:371:ILE:HB	2:B:414:VAL:HA	1.88	0.55
2:B:372:SER:O	2:B:418:ILE:HA	2.06	0.55
1:A:242:ASN:CG	1:A:282:THR:HG23	2.26	0.55
2:B:300:LEU:O	2:B:303:ALA:HB3	2.07	0.55
1:A:205:GLY:HA3	1:A:344:GLN:NE2	2.21	0.55
1:A:346:PHE:CD1	1:A:354:VAL:HG22	2.41	0.55
2:B:334:THR:CB	2:B:364:ASN:HB2	2.36	0.55
1:A:176:GLU:CD	1:A:176:GLU:H	2.09	0.55
2:B:245:THR:O	2:B:249:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:TRP:CE3	2:B:169:PHE:N	2.75	0.55
1:A:149:ALA:HA	1:A:180:GLN:HA	1.87	0.55
2:B:212:ASP:OD1	2:B:216:ASN:OD1	2.25	0.55
2:B:375:ARG:CZ	2:B:382:LEU:HD23	2.37	0.55
2:B:382:LEU:HD11	2:B:436:ASP:HA	1.87	0.55
1:A:100:THR:N	1:A:103:GLU:OE1	2.31	0.55
2:B:137:LYS:HG3	2:B:172:HIS:N	2.20	0.55
2:B:16:ILE:HG22	2:B:16:ILE:O	2.05	0.55
1:A:41:LEU:HA	1:A:69:ALA:HB3	1.87	0.55
1:A:181:ILE:HD12	1:A:237:ILE:HG13	1.89	0.55
1:A:288:LEU:C	1:A:288:LEU:HD12	2.27	0.55
2:B:343:ARG:HG3	2:B:343:ARG:NH1	2.22	0.54
2:B:66:VAL:O	2:B:213:PRO:HB3	2.06	0.54
1:A:203:THR:H	1:A:225:HIS:CD2	2.25	0.54
2:B:27:GLN:C	2:B:29:LEU:N	2.61	0.54
1:A:31:PHE:CG	2:B:489:LYS:HD3	2.41	0.54
2:B:90:ILE:CD1	2:B:147:TYR:HE2	2.20	0.54
2:B:283:LEU:HD22	2:B:287:ILE:HD11	1.88	0.54
1:A:314:ARG:O	1:A:318:SER:HB2	2.08	0.54
1:A:239:LYS:HZ2	1:A:279:PHE:HA	1.69	0.54
2:B:112:GLN:O	2:B:115:ILE:HD11	2.07	0.54
1:A:80:LYS:HD2	1:A:116:PHE:CE1	2.43	0.54
1:A:82:THR:N	1:A:85:THR:HG1	2.06	0.54
2:B:170:ARG:NH1	2:B:170:ARG:HG2	2.21	0.54
1:A:200:ALA:O	1:A:252:PHE:N	2.37	0.54
2:B:107:LYS:HZ3	2:B:424:ALA:HB1	1.72	0.54
2:B:598:LYS:HE2	2:B:613:THR:N	2.23	0.54
1:A:32:GLU:C	1:A:34:GLU:N	2.61	0.54
2:B:96:LYS:HB2	2:B:118:SER:OG	2.08	0.54
2:B:25:ASN:C	2:B:27:GLN:H	2.10	0.54
2:B:448:ILE:HG22	2:B:452:ILE:CD1	2.37	0.54
1:A:252:PHE:HA	1:A:289:GLY:CA	2.38	0.54
2:B:136:SER:CB	2:B:174:THR:HB	2.38	0.54
2:B:470:LYS:C	2:B:472:ARG:H	2.10	0.54
2:B:76:VAL:N	2:B:178:LEU:O	2.38	0.54
2:B:532:VAL:CG2	2:B:533:LYS:N	2.70	0.54
2:B:137:LYS:N	2:B:137:LYS:HD3	2.23	0.54
2:B:170:ARG:N	2:B:171:PRO:HD3	2.23	0.54
2:B:90:ILE:HG12	2:B:147:TYR:HD2	1.73	0.54
1:A:75:ALA:O	1:A:78:LEU:HB2	2.08	0.54
2:B:25:ASN:HB3	2:B:28:ILE:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:ILE:HG22	2:B:526:VAL:HG22	1.90	0.54
2:B:184:TYR:O	2:B:186:LYS:N	2.41	0.54
1:A:156:GLU:C	1:A:157:ILE:HG13	2.28	0.54
1:A:181:ILE:HD13	1:A:237:ILE:HG13	1.89	0.54
2:B:167:ASP:O	2:B:168:TRP:HB3	2.08	0.54
2:B:375:ARG:HH11	2:B:382:LEU:HD23	1.68	0.53
2:B:26:ARG:O	2:B:26:ARG:HG2	2.07	0.53
2:B:400:TRP:CE3	2:B:407:GLN:O	2.61	0.53
2:B:398:ILE:HG13	2:B:449:ASP:OD1	2.09	0.53
1:A:158:THR:O	1:A:189:GLU:HB3	2.08	0.53
2:B:373:ILE:CG1	2:B:373:ILE:O	2.55	0.53
2:B:539:ALA:HA	2:B:577:SER:HB2	1.90	0.53
2:B:544:VAL:HG22	2:B:601:GLN:HG3	1.91	0.53
1:A:18:GLU:C	1:A:20:LEU:N	2.61	0.53
1:A:305:LEU:HD21	1:A:339:LYS:N	2.23	0.53
2:B:168:TRP:O	2:B:169:PHE:CB	2.53	0.53
2:B:528:VAL:CG1	2:B:584:LEU:HD12	2.37	0.53
2:B:511:ASN:O	2:B:512:LEU:HB3	2.09	0.53
2:B:184:TYR:CE1	2:B:192:ILE:HG12	2.39	0.53
1:A:28:TYR:CE2	2:B:492:HIS:HB3	2.43	0.53
1:A:149:ALA:HA	1:A:180:GLN:HG3	1.89	0.53
2:B:78:ILE:HG22	2:B:78:ILE:O	2.07	0.53
1:A:87:PHE:HD2	1:A:111:TRP:HZ3	1.56	0.53
1:A:248:PRO:O	1:A:249:VAL:HG23	2.08	0.53
2:B:77:ILE:N	2:B:77:ILE:CD1	2.72	0.53
2:B:360:ALA:HB3	2:B:418:ILE:HG21	1.88	0.53
2:B:139:SER:CB	2:B:140:PRO:HD2	2.36	0.53
2:B:302:GLU:HA	2:B:305:GLU:HG2	1.91	0.53
1:A:181:ILE:HD11	1:A:234:THR:HA	1.91	0.53
1:A:140:PHE:O	1:A:141:HIS:CB	2.57	0.53
2:B:44:GLU:HA	2:B:44:GLU:OE2	2.09	0.53
1:A:251:VAL:HG21	1:A:263:TYR:HD1	1.74	0.53
1:A:100:THR:HG22	1:A:143:ARG:O	2.09	0.53
2:B:593:GLU:O	2:B:596:LEU:HD12	2.09	0.53
2:B:263:ARG:HD2	2:B:271:LEU:CD2	2.39	0.53
1:A:31:PHE:HB2	2:B:489:LYS:CE	2.38	0.53
1:A:83:TYR:C	1:A:85:THR:N	2.61	0.53
1:A:185:VAL:HG11	1:A:236:ARG:HB2	1.90	0.53
1:A:281:ALA:HB1	1:A:283:PRO:HD3	1.91	0.53
1:A:145:GLU:O	1:A:146:GLU:CB	2.57	0.53
2:B:515:HIS:CE1	2:B:529:ALA:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:PRO:O	2:B:292:LEU:HG	2.09	0.53
2:B:448:ILE:O	2:B:452:ILE:HG13	2.09	0.53
2:B:151:ILE:O	2:B:152:ASN:O	2.27	0.53
2:B:65:GLN:HE21	2:B:67:GLU:CG	2.22	0.52
2:B:550:CYS:O	2:B:551:LYS:CB	2.57	0.52
2:B:381:PRO:O	2:B:382:LEU:CB	2.49	0.52
2:B:61:ASP:HA	2:B:207:ARG:O	2.09	0.52
2:B:150:MET:CE	2:B:152:ASN:HB2	2.39	0.52
1:A:112:ASP:C	1:A:114:ALA:H	2.11	0.52
2:B:27:GLN:OE1	2:B:32:ASP:HB2	2.09	0.52
1:A:69:ALA:O	1:A:70:LYS:CB	2.56	0.52
2:B:557:PRO:O	2:B:558:GLU:HB2	2.09	0.52
2:B:513:LEU:HD12	2:B:513:LEU:O	2.09	0.52
2:B:65:GLN:HE21	2:B:67:GLU:HG2	1.75	0.52
2:B:348:TYR:CZ	2:B:351:ASN:HB2	2.44	0.52
1:A:108:SER:C	1:A:110:GLY:H	2.12	0.52
2:B:90:ILE:HD13	2:B:147:TYR:HE2	1.74	0.52
2:B:428:VAL:HB	2:B:430:PHE:HE2	1.73	0.52
2:B:25:ASN:O	2:B:27:GLN:N	2.41	0.52
2:B:16:ILE:O	2:B:17:SER:HB2	2.09	0.52
1:A:206:MET:O	1:A:210:LEU:HB2	2.10	0.52
2:B:418:ILE:O	2:B:418:ILE:HG23	2.09	0.52
2:B:152:ASN:O	2:B:153:THR:O	2.28	0.52
2:B:156:ASN:O	2:B:157:GLU:C	2.47	0.52
1:A:149:ALA:HB2	1:A:180:GLN:CD	2.30	0.52
2:B:534:ASN:O	2:B:534:ASN:CG	2.47	0.52
2:B:322:GLU:HG3	2:B:342:THR:HB	1.92	0.52
1:A:83:TYR:CG	2:B:488:ALA:HB1	2.44	0.52
1:A:323:GLU:OE2	1:A:328:LYS:HD2	2.09	0.52
1:A:183:PHE:N	1:A:183:PHE:CD1	2.75	0.52
2:B:337:PHE:HB2	2:B:462:TYR:CE1	2.45	0.52
2:B:392:THR:O	2:B:395:VAL:HB	2.10	0.52
2:B:493:VAL:O	2:B:495:GLU:N	2.39	0.52
2:B:190:GLN:HG2	2:B:383:LEU:CD2	2.30	0.52
2:B:453:LYS:HA	2:B:456:ALA:HB3	1.92	0.52
1:A:359:LEU:HB2	1:A:360:PRO:CD	2.40	0.52
2:B:222:ARG:NH2	2:B:332:GLU:N	2.58	0.51
2:B:559:PRO:O	2:B:560:LYS:HB2	2.10	0.51
2:B:36:ARG:HA	2:B:39:ILE:CG2	2.39	0.51
1:A:188:ILE:CG1	1:A:240:ARG:NH2	2.70	0.51
1:A:83:TYR:O	1:A:84:ALA:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:HG21	2:B:438:ILE:CD1	2.40	0.51
1:A:79:LEU:C	1:A:79:LEU:HD23	2.29	0.51
2:B:235:LEU:HB2	2:B:267:CYS:SG	2.50	0.51
1:A:149:ALA:HB2	1:A:180:GLN:OE1	2.11	0.51
2:B:496:LYS:O	2:B:497:ASP:HB2	2.09	0.51
2:B:133:LYS:HE3	2:B:146:TYR:HE1	1.74	0.51
2:B:539:ALA:HA	2:B:577:SER:CB	2.41	0.51
2:B:391:THR:O	2:B:395:VAL:HG23	2.10	0.51
1:A:31:PHE:CB	2:B:489:LYS:NZ	2.74	0.51
2:B:190:GLN:O	2:B:383:LEU:HD21	2.11	0.51
2:B:112:GLN:HB2	2:B:435:LYS:CD	2.40	0.51
2:B:78:ILE:CD1	2:B:78:ILE:N	2.74	0.51
2:B:405:LEU:HD11	2:B:415:GLY:HA3	1.91	0.51
1:A:305:LEU:CD1	1:A:305:LEU:H	1.96	0.51
2:B:90:ILE:HG22	2:B:91:PRO:CD	2.40	0.51
2:B:154:SER:O	2:B:156:ASN:N	2.44	0.51
1:A:362:ARG:HH11	1:A:362:ARG:HG3	1.75	0.51
2:B:548:LEU:O	2:B:568:TYR:N	2.45	0.51
2:B:417:VAL:O	2:B:418:ILE:HB	2.11	0.51
2:B:36:ARG:CG	2:B:384:TYR:OH	2.59	0.51
2:B:359:MET:CE	2:B:455:VAL:HG23	2.32	0.51
1:A:75:ALA:HB1	2:B:481:LYS:HD2	1.92	0.51
2:B:543:ARG:O	2:B:601:GLN:HA	2.11	0.50
2:B:396:GLU:HG2	2:B:412:ILE:N	2.26	0.50
2:B:233:GLU:HG2	2:B:234:ILE:H	1.75	0.50
2:B:477:ILE:C	2:B:479:ILE:H	2.14	0.50
2:B:451:ALA:O	2:B:454:GLU:HB2	2.11	0.50
1:A:138:GLU:HG3	1:A:236:ARG:HH12	1.76	0.50
1:A:156:GLU:O	1:A:157:ILE:CG1	2.53	0.50
2:B:528:VAL:HG12	2:B:528:VAL:O	2.11	0.50
2:B:402:GLN:O	2:B:403:TYR:HD1	1.94	0.50
2:B:423:VAL:HG21	2:B:438:ILE:HD11	1.93	0.50
2:B:532:VAL:CG2	2:B:533:LYS:H	2.25	0.50
1:A:147:ASP:OD2	1:A:147:ASP:O	2.29	0.50
1:A:235:ARG:C	1:A:237:ILE:H	2.13	0.50
1:A:31:PHE:HB2	2:B:489:LYS:HZ2	1.77	0.50
2:B:374:MET:HE2	2:B:418:ILE:HD11	1.93	0.50
2:B:354:VAL:HG22	2:B:424:ALA:HB3	1.93	0.50
2:B:65:GLN:CG	2:B:211:ILE:HG13	2.37	0.50
2:B:58:ILE:O	2:B:60:PRO:N	2.44	0.50
2:B:27:GLN:O	2:B:29:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:HIS:HA	2:B:290:HIS:CE1	2.47	0.50
1:A:98:GLY:HA3	1:A:141:HIS:ND1	2.26	0.50
2:B:171:PRO:O	2:B:172:HIS:CB	2.58	0.50
2:B:547:MET:C	2:B:548:LEU:HD12	2.32	0.50
2:B:115:ILE:O	2:B:116:GLY:O	2.29	0.50
2:B:508:ILE:HG23	2:B:509:MET:N	2.25	0.50
2:B:253:THR:CG2	2:B:254:GLU:N	2.75	0.50
1:A:106:TYR:C	1:A:108:SER:H	2.15	0.50
1:A:346:PHE:HB2	1:A:354:VAL:HG22	1.94	0.50
1:A:154:PRO:HD2	1:A:221:ALA:O	2.12	0.50
2:B:66:VAL:O	2:B:213:PRO:CD	2.61	0.49
2:B:335:VAL:CG2	2:B:360:ALA:HB1	2.39	0.49
2:B:145:HIS:HB3	2:B:147:TYR:HE1	1.73	0.49
2:B:198:ALA:HB1	2:B:376:PHE:CZ	2.46	0.49
2:B:383:LEU:C	2:B:384:TYR:HD1	2.15	0.49
2:B:235:LEU:O	2:B:267:CYS:SG	2.70	0.49
2:B:445:LYS:HA	2:B:448:ILE:HD12	1.94	0.49
2:B:428:VAL:HB	2:B:430:PHE:CE2	2.47	0.49
2:B:43:LYS:O	2:B:47:ASP:OD2	2.30	0.49
1:A:150:THR:HB	1:A:225:HIS:HB3	1.93	0.49
1:A:225:HIS:C	1:A:226:LEU:HD23	2.32	0.49
1:A:72:VAL:HG21	2:B:474:GLU:HG2	1.94	0.49
2:B:399:LYS:O	2:B:400:TRP:CG	2.66	0.49
2:B:401:LYS:O	2:B:403:TYR:N	2.46	0.49
1:A:96:ASN:O	1:A:97:ARG:O	2.31	0.49
2:B:550:CYS:N	2:B:589:GLU:OE2	2.46	0.49
2:B:112:GLN:C	2:B:115:ILE:HD11	2.32	0.49
2:B:430:PHE:CE1	2:B:435:LYS:HG2	2.47	0.49
2:B:338:ILE:CG2	2:B:339:ALA:N	2.75	0.49
1:A:125:LEU:O	1:A:128:ASP:HB2	2.12	0.49
2:B:346:ALA:HB3	2:B:353:PHE:CE1	2.47	0.49
2:B:132:THR:HG23	2:B:178:LEU:HD11	1.95	0.49
2:B:61:ASP:CB	2:B:207:ARG:HH11	2.16	0.49
1:A:149:ALA:HB2	1:A:180:GLN:HG3	1.94	0.49
2:B:342:THR:HG23	2:B:356:GLU:CG	2.41	0.49
1:A:117:LYS:HB2	1:A:117:LYS:HZ3	1.75	0.49
1:A:292:PRO:C	1:A:333:LEU:HD23	2.32	0.49
1:A:154:PRO:O	1:A:155:ILE:CG2	2.59	0.49
2:B:107:LYS:NZ	2:B:424:ALA:HB1	2.28	0.49
2:B:337:PHE:CE2	2:B:459:LEU:HA	2.47	0.49
2:B:212:ASP:CG	2:B:216:ASN:OD1	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:HG12	2:B:418:ILE:N	2.27	0.49
2:B:508:ILE:HG22	2:B:509:MET:N	2.24	0.49
2:B:348:TYR:OH	2:B:429:PRO:HD3	2.13	0.49
1:A:223:LEU:O	1:A:224:VAL:HG13	2.13	0.49
2:B:594:GLU:O	2:B:596:LEU:N	2.45	0.49
1:A:359:LEU:O	1:A:363:LEU:HB2	2.12	0.49
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.49
2:B:369:GLU:HG2	2:B:414:VAL:HG23	1.95	0.49
2:B:444:ILE:HG22	2:B:445:LYS:N	2.27	0.49
2:B:284:ASP:HB2	2:B:287:ILE:CG2	2.43	0.49
2:B:273:THR:O	2:B:277:ILE:HG13	2.12	0.49
2:B:550:CYS:HB2	2:B:589:GLU:OE2	2.13	0.49
1:A:203:THR:C	1:A:205:GLY:N	2.67	0.49
1:A:137:ARG:HB2	1:A:137:ARG:HH11	1.78	0.49
2:B:224:THR:O	2:B:226:LYS:N	2.46	0.49
2:B:396:GLU:CG	2:B:412:ILE:HG23	2.42	0.48
2:B:400:TRP:HZ3	2:B:408:PRO:CA	2.25	0.48
1:A:28:TYR:O	1:A:29:ASN:C	2.51	0.48
2:B:560:LYS:HB3	2:B:571:VAL:O	2.12	0.48
2:B:398:ILE:CG2	2:B:399:LYS:N	2.76	0.48
2:B:180:MET:CG	2:B:180:MET:O	2.59	0.48
1:A:28:TYR:CE1	2:B:489:LYS:HA	2.48	0.48
1:A:21:LEU:HD12	1:A:93:LEU:HD13	1.94	0.48
2:B:425:SER:O	2:B:427:ASN:N	2.46	0.48
1:A:198:ILE:HD12	1:A:249:VAL:CG2	2.44	0.48
1:A:331:ILE:O	1:A:334:GLN:N	2.41	0.48
2:B:75:THR:HA	2:B:178:LEU:O	2.14	0.48
2:B:193:TYR:CE1	2:B:218:GLU:HG2	2.48	0.48
1:A:85:THR:C	1:A:87:PHE:H	2.16	0.48
1:A:305:LEU:HD12	1:A:305:LEU:N	2.05	0.48
1:A:156:GLU:HA	1:A:170:CYS:HB3	1.95	0.48
1:A:288:LEU:O	1:A:288:LEU:HD12	2.13	0.48
2:B:551:LYS:HG2	2:B:552:VAL:H	1.74	0.48
2:B:449:ASP:C	2:B:451:ALA:N	2.66	0.48
1:A:151:MET:HG3	1:A:224:VAL:CG1	2.44	0.48
2:B:20:GLU:O	2:B:22:PHE:N	2.47	0.48
2:B:361:TYR:CD2	2:B:362:GLY:N	2.82	0.48
2:B:137:LYS:CE	2:B:173:GLY:H	2.26	0.48
2:B:85:ILE:HG13	2:B:90:ILE:CD1	2.44	0.48
2:B:455:VAL:C	2:B:457:ARG:H	2.17	0.48
1:A:151:MET:HG3	1:A:224:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HG2	1:A:367:GLY:O	2.13	0.48
1:A:296:VAL:HG22	1:A:337:ILE:HD11	1.94	0.48
2:B:91:PRO:O	2:B:95:ALA:HB3	2.14	0.48
2:B:46:VAL:O	2:B:50:LEU:HG	2.14	0.48
2:B:237:HIS:ND1	2:B:239:GLU:OE1	2.42	0.48
1:A:30:GLN:O	1:A:34:GLU:HB2	2.13	0.48
2:B:591:ALA:O	2:B:593:GLU:N	2.47	0.48
1:A:317:LEU:C	1:A:319:ASP:H	2.17	0.48
2:B:402:GLN:O	2:B:403:TYR:CD1	2.67	0.47
2:B:80:ASP:HB3	2:B:81:ASN:H	1.57	0.47
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.73	0.47
2:B:23:GLU:OE1	2:B:26:ARG:HD2	2.14	0.47
2:B:505:VAL:O	2:B:508:ILE:HG22	2.14	0.47
2:B:345:PRO:HB3	2:B:354:VAL:HG12	1.95	0.47
2:B:122:LEU:HD22	2:B:126:MET:CE	2.43	0.47
2:B:65:GLN:HA	2:B:211:ILE:O	2.14	0.47
2:B:338:ILE:HG22	2:B:339:ALA:N	2.30	0.47
2:B:169:PHE:CD1	2:B:169:PHE:O	2.67	0.47
2:B:53:CYS:C	2:B:55:GLU:N	2.66	0.47
1:A:122:SER:O	1:A:123:ASP:O	2.32	0.47
2:B:534:ASN:ND2	2:B:539:ALA:HB3	2.29	0.47
2:B:168:TRP:CZ3	2:B:169:PHE:HA	2.46	0.47
2:B:44:GLU:O	2:B:45:ALA:C	2.52	0.47
2:B:191:SER:OG	2:B:192:ILE:N	2.45	0.47
1:A:98:GLY:CA	1:A:141:HIS:CE1	2.97	0.47
2:B:190:GLN:HG3	2:B:194:GLU:HG2	1.95	0.47
2:B:430:PHE:CD2	2:B:435:LYS:HG2	2.49	0.47
1:A:155:ILE:HD13	1:A:222:ILE:CD1	2.45	0.47
1:A:149:ALA:HB2	1:A:180:GLN:CG	2.44	0.47
2:B:449:ASP:C	2:B:451:ALA:H	2.16	0.47
2:B:311:ALA:O	2:B:312:PRO:O	2.33	0.47
1:A:84:ALA:HB1	1:A:111:TRP:CZ2	2.50	0.47
2:B:359:MET:HB2	2:B:419:LEU:CD2	2.44	0.47
1:A:237:ILE:O	1:A:241:MET:HE2	2.14	0.47
2:B:543:ARG:O	2:B:601:GLN:CA	2.63	0.47
2:B:375:ARG:NH1	2:B:382:LEU:CD2	2.76	0.47
1:A:99:SER:HB3	1:A:103:GLU:OE1	2.15	0.47
1:A:159:GLU:HG3	1:A:160:GLN:N	2.29	0.47
1:A:338:GLY:C	1:A:339:LYS:HG3	2.35	0.47
2:B:355:VAL:HA	2:B:422:HIS:O	2.14	0.47
1:A:264:ALA:HA	1:A:267:ALA:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:SER:HB2	2:B:174:THR:HB	1.97	0.47
2:B:58:ILE:O	2:B:60:PRO:HD3	2.15	0.47
2:B:263:ARG:HG2	2:B:263:ARG:O	2.15	0.47
2:B:308:LYS:HD2	2:B:308:LYS:O	2.15	0.47
1:A:126:ILE:HD13	1:A:129:LEU:HD12	1.95	0.47
2:B:91:PRO:HB3	2:B:158:PRO:HG3	1.97	0.47
2:B:229:GLU:CG	2:B:230:PRO:HD2	2.45	0.47
1:A:279:PHE:O	1:A:280:MET:CG	2.61	0.47
2:B:561:VAL:HG21	2:B:570:TYR:HE1	1.79	0.47
1:A:260:TYR:HE1	1:A:287:PHE:CE2	2.33	0.47
2:B:53:CYS:C	2:B:55:GLU:H	2.19	0.47
2:B:281:ALA:HB2	2:B:300:LEU:HA	1.96	0.47
2:B:62:ILE:HG23	2:B:79:GLU:O	2.15	0.47
2:B:180:MET:HG2	2:B:180:MET:O	2.15	0.46
2:B:197:LYS:O	2:B:201:ILE:HG22	2.14	0.46
2:B:430:PHE:CZ	2:B:435:LYS:HE3	2.49	0.46
2:B:31:PHE:O	2:B:32:ASP:C	2.52	0.46
2:B:277:ILE:HG22	2:B:300:LEU:HD11	1.97	0.46
2:B:534:ASN:HD21	2:B:539:ALA:HB3	1.81	0.46
1:A:362:ARG:NH1	1:A:362:ARG:HG3	2.29	0.46
2:B:439:ALA:O	2:B:441:ILE:N	2.48	0.46
2:B:135:LEU:CD1	2:B:146:TYR:HB2	2.45	0.46
1:A:76:PHE:CD2	2:B:481:LYS:HE2	2.50	0.46
2:B:325:ILE:O	2:B:326:TYR:C	2.53	0.46
2:B:201:ILE:HG13	2:B:328:GLY:C	2.35	0.46
2:B:106:LEU:HB3	2:B:233:GLU:HA	1.97	0.46
1:A:231:ALA:HA	1:A:235:ARG:HH21	1.80	0.46
2:B:318:SER:OG	2:B:379:ARG:NH2	2.48	0.46
2:B:448:ILE:CG2	2:B:452:ILE:HD11	2.45	0.46
2:B:205:HIS:CG	2:B:205:HIS:O	2.68	0.46
2:B:27:GLN:C	2:B:29:LEU:H	2.17	0.46
1:A:138:GLU:CG	1:A:236:ARG:HH12	2.29	0.46
2:B:390:VAL:CG2	2:B:440:ASP:HA	2.43	0.46
2:B:457:ARG:HG3	2:B:458:LYS:N	2.30	0.46
2:B:50:LEU:O	2:B:54:GLU:HB2	2.15	0.46
2:B:348:TYR:O	2:B:349:SER:C	2.54	0.46
1:A:235:ARG:CD	1:A:265:SER:O	2.63	0.46
1:A:157:ILE:HD11	1:A:190:PHE:CD1	2.50	0.46
2:B:46:VAL:O	2:B:46:VAL:CG1	2.64	0.46
2:B:216:ASN:N	2:B:216:ASN:OD1	2.47	0.46
2:B:523:ASP:O	2:B:588:ILE:CD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD11	1:A:338:GLY:C	2.36	0.46
2:B:36:ARG:HG2	2:B:36:ARG:O	2.16	0.46
2:B:58:ILE:CG2	2:B:59:LEU:H	2.22	0.46
1:A:73:LYS:O	1:A:77:GLN:HB2	2.15	0.46
2:B:167:ASP:O	2:B:168:TRP:CB	2.64	0.46
2:B:168:TRP:HE3	2:B:169:PHE:HA	1.72	0.46
2:B:510:GLY:O	2:B:533:LYS:O	2.34	0.46
1:A:32:GLU:C	1:A:34:GLU:H	2.20	0.46
2:B:561:VAL:CG2	2:B:570:TYR:CE1	2.99	0.46
1:A:263:TYR:CE2	1:A:327:TRP:CH2	3.03	0.46
2:B:19:ALA:O	2:B:22:PHE:HB3	2.15	0.46
2:B:65:GLN:NE2	2:B:67:GLU:HG2	2.30	0.45
1:A:291:GLN:HB2	1:A:330:GLN:OE1	2.16	0.45
2:B:203:ASN:O	2:B:205:HIS:N	2.50	0.45
1:A:35:VAL:O	1:A:36:VAL:C	2.55	0.45
2:B:382:LEU:HD11	2:B:436:ASP:C	2.36	0.45
2:B:94:PHE:O	2:B:121:VAL:HG21	2.16	0.45
2:B:48:ASN:O	2:B:51:ASP:HB2	2.16	0.45
1:A:252:PHE:HA	1:A:289:GLY:HA3	1.98	0.45
1:A:76:PHE:CD2	2:B:481:LYS:NZ	2.83	0.45
1:A:360:PRO:O	1:A:363:LEU:N	2.48	0.45
2:B:512:LEU:HD11	2:B:542:PHE:CZ	2.50	0.45
2:B:396:GLU:HG2	2:B:412:ILE:H	1.82	0.45
2:B:58:ILE:O	2:B:59:LEU:C	2.55	0.45
2:B:518:ILE:HG22	2:B:526:VAL:CG1	2.44	0.45
2:B:361:TYR:O	2:B:362:GLY:O	2.35	0.45
2:B:450:LEU:O	2:B:454:GLU:HG2	2.16	0.45
1:A:29:ASN:O	1:A:31:PHE:N	2.48	0.45
2:B:18:VAL:HG23	2:B:19:ALA:H	1.81	0.45
1:A:356:GLU:O	1:A:360:PRO:CG	2.63	0.45
1:A:353:PHE:CE1	1:A:357:VAL:HG21	2.51	0.45
2:B:21:PHE:CD1	2:B:21:PHE:O	2.68	0.45
1:A:291:GLN:OE1	1:A:294:ASP:OD2	2.35	0.45
2:B:431:THR:O	2:B:432:SER:C	2.55	0.45
1:A:17:ARG:HH12	1:A:141:HIS:CD2	2.34	0.45
2:B:552:VAL:HB	2:B:587:LYS:CB	2.36	0.45
2:B:36:ARG:NH1	2:B:40:THR:OG1	2.49	0.45
1:A:155:ILE:HG22	1:A:192:LYS:O	2.17	0.45
1:A:136:GLN:O	1:A:137:ARG:C	2.55	0.45
1:A:238:ILE:HG22	1:A:282:THR:OG1	2.17	0.45
2:B:468:ASN:O	2:B:471:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLU:HB2	2:B:162:VAL:CG2	2.47	0.45
2:B:38:LEU:HA	2:B:180:MET:HE1	1.97	0.45
2:B:222:ARG:HB2	2:B:222:ARG:NH1	2.31	0.45
1:A:86:ASP:O	2:B:492:HIS:CE1	2.69	0.45
2:B:170:ARG:N	2:B:171:PRO:CD	2.79	0.45
2:B:551:LYS:HZ3	2:B:586:TYR:HB3	1.81	0.45
2:B:110:ARG:O	2:B:111:GLY:C	2.55	0.45
2:B:543:ARG:O	2:B:601:GLN:CB	2.65	0.45
2:B:234:ILE:O	2:B:234:ILE:HD12	2.17	0.45
2:B:309:ILE:CG2	2:B:310:MET:H	2.29	0.45
2:B:27:GLN:HG2	2:B:32:ASP:CB	2.41	0.45
2:B:212:ASP:CB	2:B:213:PRO:HD2	2.46	0.45
2:B:22:PHE:O	2:B:26:ARG:N	2.50	0.45
1:A:101:LEU:O	1:A:104:LEU:HB3	2.17	0.45
2:B:443:VAL:O	2:B:443:VAL:HG12	2.17	0.45
2:B:545:HIS:ND1	2:B:571:VAL:HG22	2.32	0.44
1:A:32:GLU:O	1:A:34:GLU:N	2.50	0.44
1:A:155:ILE:HD13	1:A:222:ILE:HD11	1.99	0.44
2:B:361:TYR:CD2	2:B:361:TYR:C	2.90	0.44
2:B:194:GLU:HG2	2:B:383:LEU:HD11	1.99	0.44
1:A:251:VAL:CG2	1:A:263:TYR:HD1	2.30	0.44
1:A:202:GLU:HA	1:A:225:HIS:CD2	2.52	0.44
1:A:231:ALA:C	1:A:235:ARG:HE	2.20	0.44
2:B:378:ASN:O	2:B:379:ARG:HB2	2.16	0.44
2:B:531:LYS:HG2	2:B:581:SER:CA	2.48	0.44
2:B:327:ARG:O	2:B:328:GLY:C	2.55	0.44
2:B:329:LEU:H	2:B:329:LEU:HD12	1.82	0.44
1:A:29:ASN:C	1:A:31:PHE:N	2.61	0.44
1:A:207:TYR:HE1	1:A:223:LEU:HB3	1.83	0.44
2:B:61:ASP:OD2	2:B:61:ASP:O	2.35	0.44
2:B:152:ASN:ND2	2:B:155:THR:OG1	2.50	0.44
2:B:531:LYS:HG2	2:B:581:SER:HB2	1.99	0.44
1:A:268:TYR:HB2	1:A:322:PHE:CE2	2.47	0.44
2:B:459:LEU:O	2:B:462:TYR:N	2.51	0.44
2:B:89:GLN:O	2:B:93:VAL:HG23	2.17	0.44
1:A:138:GLU:O	1:A:139:TYR:C	2.55	0.44
2:B:320:ILE:HD11	2:B:379:ARG:HH11	1.80	0.44
1:A:76:PHE:C	1:A:78:LEU:N	2.71	0.44
2:B:484:PRO:HA	2:B:487:ALA:HB3	1.99	0.44
2:B:531:LYS:HD3	2:B:581:SER:HB2	2.00	0.44
2:B:302:GLU:C	2:B:304:PHE:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:H	1:A:351:LEU:HD12	1.79	0.44
1:A:176:GLU:CD	1:A:176:GLU:N	2.71	0.44
2:B:87:ARG:HG3	2:B:88:GLU:HG3	1.98	0.44
2:B:444:ILE:O	2:B:447:GLU:HB3	2.18	0.44
2:B:198:ALA:HB1	2:B:376:PHE:HZ	1.81	0.44
2:B:195:TYR:HE1	2:B:381:PRO:HD2	1.82	0.44
2:B:440:ASP:O	2:B:440:ASP:OD1	2.35	0.44
2:B:53:CYS:SG	2:B:60:PRO:HB3	2.57	0.44
1:A:149:ALA:CB	1:A:180:GLN:HG3	2.48	0.44
2:B:37:SER:HB2	2:B:182:ALA:CB	2.45	0.44
1:A:216:ASP:OD2	1:A:216:ASP:N	2.50	0.44
2:B:521:ASN:HB2	2:B:522:GLY:H	1.50	0.44
1:A:30:GLN:O	1:A:34:GLU:CD	2.56	0.44
2:B:150:MET:HG2	2:B:151:ILE:N	2.33	0.44
1:A:231:ALA:O	1:A:235:ARG:HB2	2.18	0.44
2:B:345:PRO:CB	2:B:354:VAL:HG12	2.48	0.44
2:B:137:LYS:HG2	2:B:173:GLY:H	1.81	0.44
2:B:90:ILE:CG2	2:B:91:PRO:N	2.76	0.44
1:A:263:TYR:CZ	1:A:327:TRP:CH2	3.06	0.44
1:A:233:SER:OG	1:A:234:THR:N	2.49	0.44
1:A:330:GLN:O	1:A:333:LEU:HB3	2.18	0.44
2:B:386:GLN:O	2:B:387:GLY:C	2.56	0.44
2:B:374:MET:HE3	2:B:418:ILE:HD11	1.99	0.43
2:B:234:ILE:C	2:B:234:ILE:HD12	2.39	0.43
1:A:78:LEU:HB3	2:B:485:LYS:HZ1	1.80	0.43
1:A:117:LYS:HB2	1:A:117:LYS:HZ2	1.82	0.43
2:B:514:VAL:HA	2:B:530:ILE:HG12	2.00	0.43
2:B:603:ILE:O	2:B:604:VAL:CB	2.66	0.43
1:A:106:TYR:C	1:A:108:SER:N	2.70	0.43
2:B:42:VAL:C	2:B:44:GLU:N	2.71	0.43
1:A:201:ILE:HA	1:A:252:PHE:O	2.18	0.43
2:B:473:ARG:HE	2:B:477:ILE:HD11	1.83	0.43
2:B:30:GLY:O	2:B:31:PHE:CG	2.71	0.43
2:B:337:PHE:HE2	2:B:459:LEU:HA	1.83	0.43
2:B:195:TYR:CE1	2:B:381:PRO:HG2	2.54	0.43
1:A:155:ILE:O	1:A:170:CYS:CB	2.66	0.43
2:B:153:THR:O	2:B:154:SER:OG	2.33	0.43
1:A:125:LEU:O	1:A:128:ASP:N	2.51	0.43
1:A:217:GLU:C	1:A:219:TYR:H	2.21	0.43
2:B:400:TRP:HZ2	2:B:411:GLY:CA	2.31	0.43
2:B:64:VAL:HA	2:B:77:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:GLU:CD	2:B:239:GLU:H	2.19	0.43
2:B:82:GLY:O	2:B:172:HIS:O	2.36	0.43
2:B:355:VAL:CG2	2:B:423:VAL:HG12	2.47	0.43
2:B:65:GLN:OE1	2:B:211:ILE:HD12	2.19	0.43
1:A:84:ALA:CB	1:A:111:TRP:CE2	3.00	0.43
1:A:24:ALA:HA	1:A:27:ILE:CD1	2.48	0.43
2:B:20:GLU:O	2:B:21:PHE:C	2.56	0.43
2:B:485:LYS:C	2:B:487:ALA:N	2.72	0.43
1:A:235:ARG:C	1:A:237:ILE:N	2.71	0.43
1:A:96:ASN:O	1:A:141:HIS:NE2	2.52	0.43
2:B:158:PRO:HB2	2:B:159:ASP:H	1.58	0.43
2:B:36:ARG:HG2	2:B:36:ARG:HH11	1.84	0.43
2:B:80:ASP:O	2:B:81:ASN:HB2	2.19	0.43
1:A:161:THR:O	1:A:162:LYS:HB2	2.19	0.43
1:A:214:GLY:O	1:A:215:PHE:CB	2.65	0.43
2:B:394:ALA:CA	2:B:445:LYS:HE3	2.49	0.43
2:B:135:LEU:HD12	2:B:135:LEU:HA	1.87	0.43
1:A:79:LEU:HD22	1:A:114:ALA:CB	2.48	0.43
2:B:284:ASP:O	2:B:286:GLU:N	2.48	0.43
2:B:222:ARG:NH2	2:B:332:GLU:CB	2.67	0.43
1:A:15:LEU:HD11	1:A:141:HIS:CD2	2.53	0.43
2:B:551:LYS:HB3	2:B:570:TYR:OH	2.19	0.43
2:B:90:ILE:CD1	2:B:147:TYR:CE2	3.02	0.43
1:A:206:MET:N	1:A:344:GLN:NE2	2.66	0.43
1:A:130:GLU:CD	1:A:136:GLN:HE22	2.22	0.43
1:A:101:LEU:C	1:A:103:GLU:H	2.22	0.43
2:B:302:GLU:HA	2:B:305:GLU:HG3	2.00	0.43
2:B:502:ASN:HB3	2:B:503:PRO:HD3	2.00	0.43
2:B:541:SER:HA	2:B:575:SER:OG	2.19	0.43
2:B:411:GLY:O	2:B:412:ILE:CG1	2.57	0.43
2:B:203:ASN:O	2:B:204:PRO:C	2.57	0.43
2:B:500:ASP:HB3	2:B:503:PRO:HD3	2.01	0.43
1:A:145:GLU:O	1:A:146:GLU:HG3	2.18	0.43
1:A:107:ILE:HG22	1:A:107:ILE:O	2.19	0.43
2:B:357:VAL:CG2	2:B:421:ILE:HG12	2.48	0.43
1:A:32:GLU:O	1:A:35:VAL:N	2.52	0.43
1:A:85:THR:C	1:A:87:PHE:N	2.72	0.43
1:A:96:ASN:O	1:A:97:ARG:C	2.57	0.43
2:B:375:ARG:HD2	2:B:382:LEU:CD2	2.45	0.43
2:B:382:LEU:HD11	2:B:436:ASP:O	2.19	0.43
2:B:314:THR:O	2:B:316:CYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:LEU:HB2	2:B:267:CYS:H	1.84	0.43
2:B:204:PRO:HA	2:B:222:ARG:HD3	2.01	0.42
2:B:61:ASP:OD1	2:B:207:ARG:NH1	2.52	0.42
2:B:337:PHE:HB2	2:B:462:TYR:CD1	2.54	0.42
1:A:79:LEU:HD21	1:A:114:ALA:HB2	1.98	0.42
1:A:118:GLU:C	1:A:120:GLY:N	2.73	0.42
2:B:300:LEU:HD12	2:B:303:ALA:HB3	2.01	0.42
2:B:122:LEU:HD22	2:B:126:MET:HE1	2.00	0.42
2:B:376:PHE:CD2	2:B:381:PRO:HA	2.54	0.42
2:B:389:CYS:O	2:B:390:VAL:C	2.56	0.42
2:B:48:ASN:ND2	2:B:117:ILE:HG12	2.32	0.42
2:B:117:ILE:O	2:B:121:VAL:HG23	2.20	0.42
2:B:475:LYS:O	2:B:479:ILE:HG13	2.18	0.42
2:B:479:ILE:HG23	2:B:505:VAL:HG11	2.01	0.42
2:B:576:ALA:HB2	2:B:582:LYS:CE	2.49	0.42
1:A:268:TYR:HB3	1:A:269:GLY:H	1.61	0.42
2:B:263:ARG:HD2	2:B:271:LEU:CG	2.47	0.42
1:A:135:LEU:CB	1:A:140:PHE:HE1	2.30	0.42
2:B:81:ASN:O	2:B:81:ASN:CG	2.56	0.42
1:A:155:ILE:O	1:A:155:ILE:HG13	2.20	0.42
2:B:479:ILE:HG22	2:B:479:ILE:O	2.19	0.42
2:B:353:PHE:CA	2:B:424:ALA:O	2.61	0.42
2:B:576:ALA:CB	2:B:582:LYS:HE3	2.48	0.42
1:A:102:ARG:O	1:A:106:TYR:HD1	2.01	0.42
2:B:382:LEU:HD11	2:B:436:ASP:CA	2.49	0.42
2:B:184:TYR:CE2	2:B:212:ASP:HB2	2.54	0.42
2:B:65:GLN:OE1	2:B:211:ILE:CD1	2.68	0.42
1:A:300:LEU:HD11	1:A:346:PHE:HE2	1.84	0.42
2:B:507:LYS:HA	2:B:533:LYS:HD2	2.01	0.42
1:A:169:HIS:HD2	1:A:172:LYS:H	1.68	0.42
1:A:20:LEU:C	1:A:22:GLU:N	2.73	0.42
2:B:232:GLU:CD	2:B:316:CYS:CA	2.73	0.42
2:B:342:THR:HA	2:B:356:GLU:HG2	2.02	0.42
2:B:222:ARG:HB2	2:B:222:ARG:HH11	1.85	0.42
2:B:490:VAL:HG21	2:B:498:VAL:HG22	2.02	0.42
2:B:455:VAL:HG23	2:B:456:ALA:N	2.35	0.42
2:B:455:VAL:O	2:B:456:ALA:C	2.58	0.42
2:B:453:LYS:CE	2:B:457:ARG:HH21	2.29	0.42
1:A:155:ILE:C	1:A:170:CYS:HB3	2.40	0.42
2:B:18:VAL:CG1	2:B:156:ASN:OD1	2.68	0.42
1:A:169:HIS:O	1:A:174:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:VAL:O	2:B:46:VAL:HG12	2.20	0.42
1:A:194:ASP:N	1:A:194:ASP:OD1	2.53	0.42
2:B:65:GLN:HG2	2:B:66:VAL:N	2.30	0.42
2:B:405:LEU:HD22	2:B:417:VAL:HG21	2.02	0.42
2:B:190:GLN:NE2	2:B:383:LEU:HD11	2.35	0.42
1:A:78:LEU:O	1:A:79:LEU:C	2.57	0.42
2:B:232:GLU:OE2	2:B:316:CYS:CA	2.65	0.42
1:A:206:MET:HG2	1:A:343:GLN:NE2	2.34	0.42
2:B:21:PHE:CD1	2:B:21:PHE:C	2.92	0.42
2:B:500:ASP:HB3	2:B:503:PRO:CD	2.50	0.42
1:A:26:LYS:HB2	1:A:26:LYS:HE3	1.78	0.42
2:B:445:LYS:C	2:B:447:GLU:N	2.73	0.41
2:B:359:MET:HE1	2:B:455:VAL:CG2	2.34	0.41
2:B:480:THR:O	2:B:480:THR:HG22	2.20	0.41
2:B:323:ASP:O	2:B:326:TYR:HB3	2.19	0.41
1:A:71:THR:HA	2:B:478:ILE:HD13	2.02	0.41
1:A:180:GLN:O	1:A:182:PRO:HD3	2.19	0.41
2:B:531:LYS:CG	2:B:581:SER:HB2	2.49	0.41
2:B:34:ALA:N	2:B:35:PRO:CD	2.83	0.41
2:B:329:LEU:O	2:B:330:GLU:C	2.59	0.41
2:B:39:ILE:HG23	2:B:40:THR:N	2.35	0.41
2:B:307:VAL:CG1	2:B:307:VAL:O	2.67	0.41
2:B:309:ILE:O	2:B:310:MET:O	2.37	0.41
2:B:434:SER:O	2:B:435:LYS:C	2.59	0.41
2:B:263:ARG:HH11	2:B:271:LEU:HD11	1.83	0.41
1:A:118:GLU:O	1:A:120:GLY:N	2.54	0.41
1:A:309:ASP:O	1:A:312:ALA:HB3	2.20	0.41
2:B:543:ARG:HB2	2:B:602:LEU:HB2	2.03	0.41
2:B:131:HIS:HB2	2:B:132:THR:H	1.74	0.41
1:A:185:VAL:HG21	1:A:236:ARG:CB	2.40	0.41
2:B:417:VAL:O	2:B:418:ILE:CB	2.68	0.41
1:A:41:LEU:HD22	1:A:68:SER:O	2.20	0.41
2:B:478:ILE:C	2:B:479:ILE:HG13	2.41	0.41
1:A:159:GLU:HG3	1:A:160:GLN:H	1.83	0.41
2:B:343:ARG:NH1	2:B:447:GLU:OE2	2.54	0.41
2:B:178:LEU:HD12	2:B:178:LEU:HA	1.83	0.41
1:A:135:LEU:O	1:A:140:PHE:HE1	2.03	0.41
2:B:30:GLY:O	2:B:31:PHE:CD1	2.73	0.41
2:B:110:ARG:HB3	2:B:111:GLY:H	1.51	0.41
1:A:138:GLU:HB2	1:A:236:ARG:HH12	1.86	0.41
2:B:118:SER:O	2:B:121:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HA	1:A:171:GLN:HA	2.02	0.41
1:A:158:THR:H	1:A:189:GLU:HB3	1.84	0.41
2:B:483:LEU:HB3	2:B:484:PRO:CD	2.51	0.41
1:A:162:LYS:O	1:A:163:ARG:C	2.58	0.41
1:A:180:GLN:O	1:A:181:ILE:C	2.58	0.41
1:A:215:PHE:CE2	1:A:219:TYR:HD2	2.38	0.41
1:A:321:ARG:HA	1:A:321:ARG:HD3	1.89	0.41
2:B:556:LYS:N	2:B:556:LYS:HD3	2.36	0.41
2:B:167:ASP:O	2:B:168:TRP:CD1	2.73	0.41
2:B:381:PRO:HB2	2:B:382:LEU:H	1.61	0.41
2:B:44:GLU:O	2:B:47:ASP:N	2.42	0.41
1:A:31:PHE:HE1	1:A:32:GLU:HG3	1.77	0.41
2:B:365:LEU:CD1	2:B:417:VAL:O	2.69	0.41
2:B:188:ARG:CG	2:B:189:ARG:H	2.32	0.41
2:B:309:ILE:CG2	2:B:310:MET:N	2.81	0.41
2:B:153:THR:O	2:B:155:THR:N	2.54	0.41
1:A:240:ARG:HG2	1:A:240:ARG:O	2.20	0.41
2:B:615:ALA:O	2:B:616:LYS:CB	2.68	0.41
2:B:544:VAL:HG12	2:B:544:VAL:O	2.19	0.41
1:A:20:LEU:HB2	1:A:135:LEU:HD11	2.01	0.41
2:B:561:VAL:HG22	2:B:570:TYR:CE1	2.56	0.41
2:B:307:VAL:CG2	2:B:309:ILE:HD11	2.34	0.41
1:A:346:PHE:CB	1:A:354:VAL:HG22	2.50	0.41
1:A:300:LEU:HD11	1:A:346:PHE:CD2	2.56	0.41
2:B:345:PRO:HB3	2:B:354:VAL:CG1	2.51	0.41
2:B:27:GLN:C	2:B:27:GLN:HE21	2.24	0.41
1:A:340:LYS:O	1:A:341:ALA:HB2	2.21	0.41
2:B:267:CYS:O	2:B:268:LYS:C	2.59	0.41
2:B:512:LEU:N	2:B:512:LEU:HD23	2.36	0.41
2:B:161:LEU:O	2:B:162:VAL:HG22	2.20	0.41
2:B:470:LYS:O	2:B:472:ARG:N	2.50	0.41
2:B:462:TYR:O	2:B:466:GLN:N	2.28	0.41
1:A:193:HIS:CG	1:A:193:HIS:O	2.73	0.41
2:B:262:LEU:HD13	2:B:274:ALA:HA	2.02	0.41
1:A:245:LEU:HD13	1:A:247:ILE:HD12	2.02	0.41
2:B:36:ARG:HB2	2:B:384:TYR:OH	2.21	0.41
2:B:355:VAL:HG13	2:B:422:HIS:O	2.21	0.41
2:B:390:VAL:HB	2:B:438:ILE:HB	2.02	0.41
1:A:68:SER:O	1:A:69:ALA:HB3	2.20	0.41
1:A:72:VAL:HA	2:B:481:LYS:HZ2	1.86	0.41
2:B:25:ASN:C	2:B:27:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:PHE:CE2	2:B:123:TYR:CG	3.09	0.41
1:A:357:VAL:O	1:A:361:ASN:HB2	2.20	0.41
1:A:245:LEU:HB3	1:A:247:ILE:CD1	2.51	0.41
2:B:202:VAL:C	2:B:204:PRO:CD	2.85	0.40
1:A:21:LEU:HD23	1:A:21:LEU:C	2.41	0.40
2:B:417:VAL:CG1	2:B:418:ILE:H	2.24	0.40
2:B:309:ILE:O	2:B:310:MET:C	2.59	0.40
2:B:80:ASP:HB2	2:B:174:THR:H	1.85	0.40
1:A:258:TRP:CZ3	1:A:261:ARG:CZ	3.05	0.40
2:B:516:ARG:NH2	2:B:546:GLU:OE1	2.54	0.40
1:A:17:ARG:NH1	1:A:17:ARG:HG3	2.36	0.40
2:B:44:GLU:OE1	2:B:116:GLY:HA2	2.20	0.40
2:B:96:LYS:CB	2:B:118:SER:OG	2.70	0.40
2:B:425:SER:O	2:B:426:ILE:C	2.59	0.40
2:B:42:VAL:C	2:B:44:GLU:H	2.24	0.40
2:B:484:PRO:O	2:B:487:ALA:HB3	2.21	0.40
1:A:231:ALA:HA	1:A:235:ARG:CZ	2.51	0.40
2:B:576:ALA:HB1	2:B:580:SER:CB	2.48	0.40
2:B:246:LEU:O	2:B:250:LEU:HG	2.22	0.40
2:B:58:ILE:O	2:B:60:PRO:CD	2.68	0.40
2:B:148:GLU:HG3	2:B:162:VAL:HG21	2.02	0.40
2:B:208:ILE:HB	2:B:220:PHE:HB2	2.04	0.40
2:B:497:ASP:O	2:B:499:PRO:CD	2.51	0.40
1:A:76:PHE:CE2	2:B:481:LYS:HE2	2.56	0.40
1:A:235:ARG:O	1:A:237:ILE:N	2.54	0.40
2:B:320:ILE:HA	2:B:320:ILE:HD13	1.91	0.40
2:B:333:THR:HB	2:B:334:THR:H	1.47	0.40
2:B:284:ASP:C	2:B:286:GLU:H	2.25	0.40
2:B:224:THR:HG22	2:B:224:THR:O	2.22	0.40
2:B:401:LYS:HZ2	2:B:406:ASN:CG	2.24	0.40
2:B:65:GLN:HB3	2:B:77:ILE:HD13	2.02	0.40
2:B:425:SER:OG	2:B:427:ASN:O	2.31	0.40
2:B:430:PHE:CD1	2:B:435:LYS:HG2	2.57	0.40
1:A:346:PHE:HB2	1:A:354:VAL:CG2	2.52	0.40
1:A:80:LYS:HG2	1:A:114:ALA:O	2.21	0.40
1:A:147:ASP:HB2	1:A:180:GLN:NE2	2.37	0.40
1:A:357:VAL:O	1:A:360:PRO:HG2	2.21	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	303/369 (82%)	163 (54%)	78 (26%)	62 (20%)	0 2
2	B	566/621 (91%)	339 (60%)	122 (22%)	105 (19%)	0 3
All	All	869/990 (88%)	502 (58%)	200 (23%)	167 (19%)	0 3

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	VAL
1	A	97	ARG
1	A	112	ASP
1	A	113	TYR
1	A	115	LYS
1	A	123	ASP
1	A	124	ARG
1	A	137	ARG
1	A	146	GLU
1	A	160	GLN
1	A	192	LYS
1	A	215	PHE
1	A	280	MET
1	A	282	THR
1	A	300	LEU
2	B	12	LYS
2	B	14	LYS
2	B	26	ARG
2	B	58	ILE
2	B	66	VAL
2	B	81	ASN
2	B	115	ILE
2	B	116	GLY
2	B	117	ILE

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Mol	Chain	Res	Type
2	B	131	HIS
2	B	132	THR
2	B	152	ASN
2	B	153	THR
2	B	158	PRO
2	B	159	ASP
2	B	168	TRP
2	B	169	PHE
2	B	171	PRO
2	B	172	HIS
2	B	185	VAL
2	B	189	ARG
2	B	190	GLN
2	B	224	THR
2	B	225	ASP
2	B	251	HIS
2	B	267	CYS
2	B	310	MET
2	B	349	SER
2	B	362	GLY
2	B	367	LYS
2	B	381	PRO
2	B	382	LEU
2	B	385	GLN
2	B	400	TRP
2	B	418	ILE
2	B	440	ASP
2	B	491	ALA
2	B	494	LEU
2	B	496	LYS
2	B	498	VAL
2	B	551	LYS
2	B	560	LYS
2	B	589	GLU
2	B	592	SER
2	B	603	ILE
1	A	16	ALA
1	A	39	VAL
1	A	70	LYS
1	A	83	TYR
1	A	84	ALA
1	A	85	THR

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Mol	Chain	Res	Type
1	A	119	GLN
1	A	141	HIS
1	A	149	ALA
1	A	150	THR
1	A	155	ILE
1	A	175	GLY
1	A	183	PHE
1	A	205	GLY
1	A	227	LYS
1	A	232	ARG
1	A	233	SER
1	A	254	ASP
1	A	290	LEU
1	A	299	GLU
1	A	366	MET
2	B	17	SER
2	B	31	PHE
2	B	52	ALA
2	B	54	GLU
2	B	104	HIS
2	B	111	GLY
2	B	114	GLY
2	B	140	PRO
2	B	155	THR
2	B	289	PRO
2	B	312	PRO
2	B	365	LEU
2	B	403	TYR
2	B	431	THR
2	B	435	LYS
2	B	456	ALA
2	B	497	ASP
2	B	500	ASP
2	B	512	LEU
2	B	524	GLY
2	B	546	GLU
2	B	593	GLU
2	B	598	LYS
2	B	604	VAL
1	A	102	ARG
1	A	144	PRO
1	A	203	THR

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Mol	Chain	Res	Type
1	A	341	ALA
1	A	342	GLU
2	B	23	GLU
2	B	32	ASP
2	B	45	ALA
2	B	238	PRO
2	B	426	ILE
2	B	432	SER
2	B	449	ASP
2	B	454	GLU
2	B	586	TYR
2	B	595	GLU
2	B	596	LEU
1	A	37	PRO
1	A	42	PRO
1	A	86	ASP
1	A	96	ASN
1	A	114	ALA
1	A	184	ASN
1	A	234	THR
1	A	236	ARG
1	A	268	TYR
2	B	21	PHE
2	B	80	ASP
2	B	113	GLN
2	B	188	ARG
2	B	250	LEU
2	B	285	PRO
2	B	333	THR
2	B	402	GLN
2	B	471	LYS
2	B	499	PRO
2	B	521	ASN
2	B	557	PRO
2	B	558	GLU
1	A	30	GLN
1	A	89	ILE
1	A	212	GLU
1	A	218	ALA
1	A	336	ASP
2	B	15	SER
2	B	204	PRO

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Mol	Chain	Res	Type
2	B	313	PRO
2	B	334	THR
2	B	433	GLU
2	B	550	CYS
2	B	588	ILE
1	A	190	PHE
1	A	320	PRO
2	B	483	LEU
2	B	412	ILE
2	B	417	VAL
1	A	182	PRO
1	A	337	ILE
2	B	559	PRO
1	A	295	ILE
1	A	292	PRO
2	B	478	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/315 (85%)	240 (90%)	28 (10%)	9 40
2	B	486/527 (92%)	428 (88%)	58 (12%)	6 34
All	All	754/842 (90%)	668 (89%)	86 (11%)	7 36

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	28	TYR
1	A	76	PHE
1	A	111	TRP
1	A	118	GLU
1	A	140	PHE
1	A	143	ARG

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	174	VAL
1	A	176	GLU
1	A	182	PRO
1	A	183	PHE
1	A	187	ASN
1	A	194	ASP
1	A	203	THR
1	A	210	LEU
1	A	215	PHE
1	A	219	TYR
1	A	260	TYR
1	A	261	ARG
1	A	268	TYR
1	A	286	LYS
1	A	305	LEU
1	A	319	ASP
1	A	322	PHE
1	A	325	ASP
1	A	352	ASP
1	A	355	THR
2	B	21	PHE
2	B	27	GLN
2	B	29	LEU
2	B	58	ILE
2	B	64	VAL
2	B	79	GLU
2	B	83	PRO
2	B	89	GLN
2	B	97	LEU
2	B	99	TYR
2	B	109	SER
2	B	115	ILE
2	B	117	ILE
2	B	121	VAL
2	B	137	LYS
2	B	159	ASP
2	B	161	LEU
2	B	166	ARG
2	B	169	PHE
2	B	170	ARG
2	B	171	PRO

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Mol	Chain	Res	Type
2	B	175	GLN
2	B	178	LEU
2	B	179	GLU
2	B	185	VAL
2	B	210	LEU
2	B	214	ASP
2	B	216	ASN
2	B	218	GLU
2	B	261	PHE
2	B	308	LYS
2	B	310	MET
2	B	315	ASP
2	B	333	THR
2	B	334	THR
2	B	366	PRO
2	B	373	ILE
2	B	383	LEU
2	B	391	THR
2	B	397	ASP
2	B	402	GLN
2	B	403	TYR
2	B	436	ASP
2	B	461	HIS
2	B	473	ARG
2	B	492	HIS
2	B	502	ASN
2	B	513	LEU
2	B	516	ARG
2	B	521	ASN
2	B	527	ASP
2	B	540	TYR
2	B	542	PHE
2	B	548	LEU
2	B	551	LYS
2	B	556	LYS
2	B	564	MET
2	B	599	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	90	ASN
1	A	119	GLN
1	A	187	ASN
1	A	193	HIS
1	A	332	GLN
1	A	344	GLN
2	B	25	ASN
2	B	48	ASN
2	B	81	ASN
2	B	152	ASN
2	B	175	GLN
2	B	190	GLN
2	B	378	ASN
2	B	406	ASN
2	B	502	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 carbohydrates 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	315/369 (85%)	0.01	4 (1%)	79	70	139, 217, 258, 265	0
2	B	582/621 (93%)	-0.02	3 (0%)	91	88	93, 175, 248, 265	0
All	All	897/990 (90%)	-0.01	7 (0%)	87	82	93, 192, 254, 265	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ILE	2.2
1	A	260	TYR	2.1
1	A	143	ARG	2.1
2	B	359	MET	2.1
1	A	201	ILE	2.0
2	B	423	VAL	2.0
2	B	294	ARG	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.