Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:15 PM GMT

PDB ID	:	1JIB
Title	:	Complex of Alpha-amylase II (TVA II) from Thermoactinomyces vulgaris R-47 with Maltotetraose Based on a Crystal Soaked with Maltohexaose.
Authors	:	Yokota, T.; Tonozuka, T.; Shimura, Y.; Ichikawa, K.; Kamitori, S.; Sakano, Y.
Deposited on	:	2001-07-02
Resolution	:	3.30 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 (i) symbol.

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

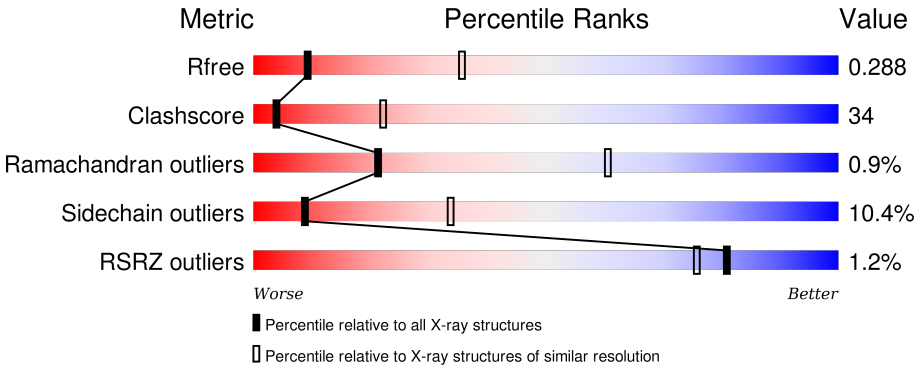
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	585	% 46% 47% 6%
1	B	585	2% 43% 49% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9642 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.

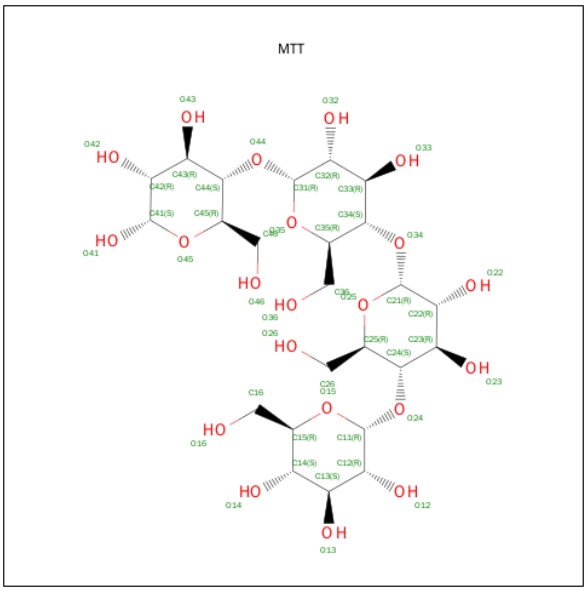
- Molecule 1 is a protein called NEOPULLULANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	ENGINEERED	UNP Q08751
B	325	ASN	ASP	ENGINEERED	UNP Q08751

- Molecule 2 is MALTOTETRAOSE (three-letter code: MTT) (formula: $C_{24}H_{42}O_{21}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			45	24	21		

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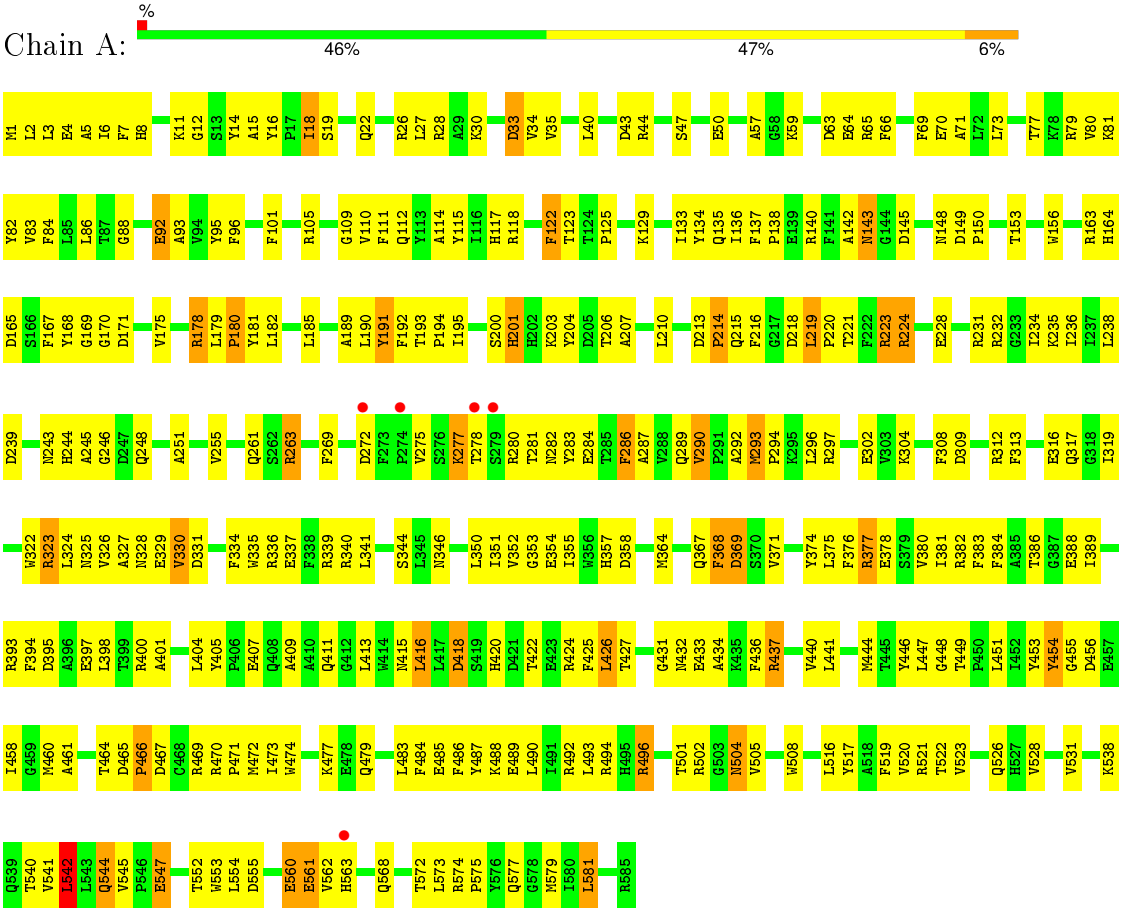
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			45	24	21		

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.

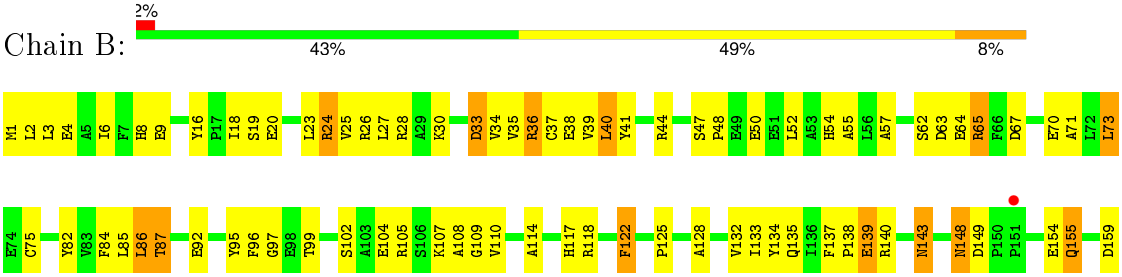
- Molecule 1: NEOPULLULANASE

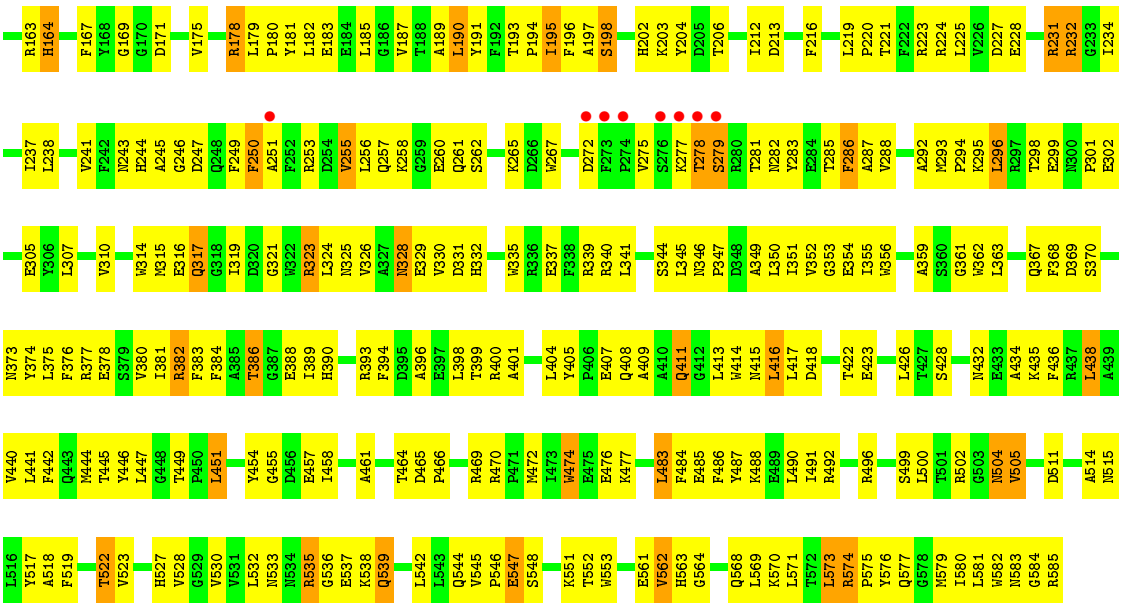
Chain A:



- Molecule 1: NEOPULLULANASE

Chain B:




R163 H164 F167 Y168 G169 G170 D171 V175 R178 L179 P180 Y181 L182 E183 E184 L185 G186 V187 T188 A189 L190 Y191 F192 T193 P194 I195 F196 A197 S198 H202 K203 Y204 D205 T206 I212 D213 F216 L219 P220 T221 F222 R223 R224 L225 V226 D227 E228 R231 R232 G233 I234
I237 L238 V241 F242 N243 H244 A245 G246 D247 Q248 F249 P250 A251 F252 R253 D254 V255 L256 Q257 K258 G259 E260 Q261 S262 K265 D266 W267 D272 F273 P274 V275 S276 K277 T278 S279 R280 T281 N282 Y283 E284 T285 P286 A287 V288 A292 M293 P294 K295 L296 R297 T298 E299 N300 P301 E302
E305 Y306 L307 V310 W314 N315 E316 Q317 G318 I319 D320 G321 W322 R323 L324 N325 V326 A327 N328 E329 V330 D331 H332 W335 R336 E337 F338 R339 R340 L341 S344 L345 N346 P347 D348 A349 L350 I351 V352 G353 E354 I355 W356 A359 S360 G361 W362 L363 Q367 F368 D369 S370
N373 Y374 L375 F376 R377 E378 S379 V380 I381 R382 F383 F384 A385 T386 G387 E388 I389 H390 R393 F394 D395 A396 E397 L398 T399 R400 A401 L404 Y405 P406 E407 Q408 A409 A410 Q411 G412 L413 W414 N415 L416 L417 D418 T422 E423 L426 T427 S428 N432 E433 A434 K435 F436 R437 L438 A439
V440 L441 F442 Q443 M444 T445 Y446 L447 G448 T449 P450 L451 Y454 G455 D456 E457 I458 A461 T464 D465 P466 R469 R470 P471 M472 I473 W474 E475 E476 K477 L483 F484 E485 F486 Y487 K488 E489 L490 I491 R492 R496 S499 L500 T501 R502 G503 N504 V505 D511 A514 N515
L516 Y517 A518 F519 T522 V523 H527 V528 G529 V530 V531 L532 N533 N534 R535 G536 E537 K538 Q539 L542 L543 Q544 V545 P546 E547 S548 K551 T552 W553 E561 V562 H563 G564 Q568 L569 K570 L571 T572 L573 R574 P575 Y576 Q577 G578 M579 I580 L581 W582 N583 G584 R585

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.87Å 117.32Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 3.30 39.68 – 3.28	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.60-3.30) 94.6 (39.68-3.28)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.304 0.205 , 0.288	Depositor DCC
R_{free} test set	2182 reflections (9.95%)	DCC
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.8	EDS
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -k,-h,-l 0.008 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 22115 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9642	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MTT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/4906	0.70	2/6641 (0.0%)
1	B	0.46	0/4906	0.69	0/6641
All	All	0.47	0/9812	0.70	2/13282 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	ARG	N-CA-C	-6.32	93.94	111.00
1	A	542	LEU	CA-CB-CG	5.32	127.55	115.30

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	4776	0	4609	332	0
1	B	4776	0	4609	342	0
2	A	45	0	42	2	0
2	B	45	0	42	2	0
All	All	9642	0	9302	653	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 34.

All (653) 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:275:VAL:HA	1:A:282:ASN:HD21	1.14	1.08
1:A:552:THR:HG23	1:A:562:VAL:HG11	1.19	1.06
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.38	1.03
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.40	1.01
1:B:552:THR:HG22	1:B:562:VAL:HG23	1.38	1.01
1:A:553:TRP:H	1:A:562:VAL:HG12	1.27	0.95
1:B:155:GLN:HA	1:B:155:GLN:HE21	1.31	0.94
1:B:416:LEU:H	1:B:416:LEU:HD23	1.32	0.93
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.49	0.93
1:A:540:THR:HG22	1:A:572:THR:HG23	1.49	0.93
1:B:426:LEU:HD23	1:B:461:ALA:HB2	1.47	0.93
1:A:165:ASP:HA	1:A:201:HIS:NE2	1.84	0.92
1:B:301:PRO:O	1:B:305:GLU:HG2	1.70	0.90
1:A:246:GLY:HA3	1:A:248:GLN:NE2	1.85	0.90
1:B:552:THR:CG2	1:B:562:VAL:HG23	2.01	0.90
1:A:207:ALA:HA	1:A:248:GLN:HG2	1.55	0.89
1:A:552:THR:HA	1:A:562:VAL:HB	1.53	0.89
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.54	0.89
1:B:190:LEU:HD22	1:B:234:ILE:HG21	1.57	0.87
1:A:328:ASN:HD22	1:A:355:ILE:HG23	1.39	0.87
1:B:356:TRP:HE3	1:B:374:TYR:HB2	1.38	0.86
1:A:552:THR:HG23	1:A:562:VAL:CG1	2.04	0.85
1:A:401:ALA:O	1:A:404:LEU:HB2	1.76	0.84
1:A:18:ILE:HD11	1:A:22:GLN:HB2	1.59	0.84
1:B:137:PHE:HD2	1:B:193:THR:HG21	1.41	0.84
1:B:26:ARG:HG2	1:B:70:GLU:HG3	1.60	0.84
1:A:377:ARG:NH1	1:A:381:ILE:HD11	1.92	0.83
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.58	0.83
1:A:552:THR:CG2	1:A:562:VAL:HG11	2.08	0.82
1:B:223:ARG:HD2	1:B:317:GLN:HG3	1.62	0.82
1:B:224:ARG:HH21	1:B:227:ASP:CB	1.92	0.82
1:B:488:LYS:HB3	1:B:492:ARG:HH11	1.45	0.81
1:B:394:PHE:CE2	1:B:398:LEU:HD11	2.15	0.81
1:A:246:GLY:HA3	1:A:248:GLN:HE22	1.43	0.80
1:A:275:VAL:HA	1:A:282:ASN:ND2	1.95	0.80
1:B:243:ASN:ND2	1:B:329:GLU:HB2	1.96	0.80
1:B:244:HIS:HD2	1:B:293:MET:HB3	1.46	0.80
1:A:309:ASP:HA	1:A:312:ARG:HD2	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLN:HE21	1:A:544:GLN:HA	1.47	0.79
1:B:36:ARG:HH21	1:B:36:ARG:HG2	1.46	0.79
1:A:145:ASP:O	1:A:148:ASN:ND2	2.12	0.79
1:A:340:ARG:NH1	1:B:340:ARG:HH22	1.80	0.78
1:A:553:TRP:N	1:A:562:VAL:HG12	1.96	0.78
1:A:140:ARG:HG2	1:A:469:ARG:O	1.84	0.78
1:A:562:VAL:O	1:A:562:VAL:HG23	1.83	0.78
1:B:416:LEU:CD2	1:B:416:LEU:H	1.95	0.78
1:A:538:LYS:HB2	1:A:573:LEU:O	1.82	0.78
1:A:182:LEU:HD12	1:A:182:LEU:N	1.99	0.77
1:A:337:GLU:HA	1:A:340:ARG:HD2	1.67	0.76
1:B:41:TYR:HB3	1:B:82:TYR:HB3	1.67	0.76
1:B:326:VAL:HG12	1:B:329:GLU:HG3	1.67	0.76
1:A:194:PRO:HD3	1:A:239:ASP:OD2	1.84	0.76
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.68	0.76
1:B:411:GLN:OE1	1:B:502:ARG:HA	1.85	0.75
1:A:382:ARG:NH2	1:A:397:GLU:OE1	2.19	0.75
1:A:330:VAL:HG13	1:A:335:TRP:NE1	2.02	0.75
1:A:182:LEU:H	1:A:182:LEU:HD12	1.50	0.75
1:B:99:THR:HB	1:B:109:GLY:HA3	1.68	0.75
1:A:340:ARG:HH12	1:B:340:ARG:HH22	1.33	0.75
1:B:352:VAL:HG22	1:B:370:SER:HB3	1.69	0.74
1:B:275:VAL:HG12	1:B:282:ASN:HB2	1.70	0.74
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.70	0.74
1:B:224:ARG:HH21	1:B:227:ASP:HB2	1.53	0.73
1:A:542:LEU:O	1:A:542:LEU:HD13	1.88	0.73
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.69	0.73
1:B:140:ARG:HD2	1:B:469:ARG:O	1.87	0.73
1:A:148:ASN:ND2	1:A:171:ASP:OD2	2.21	0.73
1:B:137:PHE:CD2	1:B:193:THR:HG21	2.24	0.72
1:B:2:LEU:HD12	1:B:30:LYS:HD2	1.72	0.72
1:B:212:ILE:H	1:B:212:ILE:HD12	1.54	0.72
1:B:573:LEU:N	1:B:573:LEU:HD22	2.05	0.72
1:B:135:GLN:HG3	1:B:191:TYR:CD2	2.24	0.72
1:B:355:ILE:HD13	1:B:362:TRP:CE3	2.24	0.72
1:B:175:VAL:HG12	1:B:225:LEU:HD11	1.72	0.72
1:B:180:PRO:HG3	1:B:232:ARG:NH2	2.05	0.71
1:B:193:THR:HB	1:B:194:PRO:HD2	1.71	0.71
1:A:340:ARG:HH12	1:B:340:ARG:HH12	1.36	0.71
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.73	0.71
1:A:277:LYS:HE2	1:A:278:THR:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:HH12	1:B:340:ARG:NH2	1.89	0.70
1:B:244:HIS:CD2	1:B:293:MET:HB3	2.26	0.70
1:B:547:GLU:HG2	1:B:551:LYS:HD3	1.71	0.70
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.21	0.70
1:A:193:THR:CG2	1:A:194:PRO:HD2	2.20	0.70
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.27	0.69
1:B:238:LEU:HD11	1:B:319:ILE:HG21	1.73	0.69
1:A:182:LEU:HD23	1:A:190:LEU:HD21	1.73	0.69
1:B:584:GLY:O	1:B:585:ARG:HD2	1.91	0.69
1:B:195:ILE:O	1:B:195:ILE:HG12	1.92	0.68
1:A:115:TYR:CE1	1:B:295:LYS:HE2	2.29	0.68
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.29	0.68
1:A:277:LYS:HD3	1:A:277:LYS:H	1.59	0.68
1:B:350:LEU:HD12	1:B:351:ILE:H	1.59	0.68
1:B:198:SER:HB2	1:B:203:LYS:HG3	1.76	0.68
1:A:340:ARG:HH12	1:B:340:ARG:NH1	1.91	0.68
1:B:164:HIS:CE1	1:B:466:PRO:HD3	2.30	0.67
1:A:246:GLY:HA2	1:A:292:ALA:O	1.95	0.67
1:B:436:PHE:O	1:B:440:VAL:HG13	1.94	0.67
1:A:164:HIS:CD2	1:A:164:HIS:H	2.11	0.67
1:A:193:THR:HG22	1:A:194:PRO:HD2	1.76	0.67
1:B:432:ASN:OD1	1:B:434:ALA:HB3	1.94	0.66
1:B:562:VAL:O	1:B:562:VAL:HG22	1.95	0.66
1:A:394:PHE:O	1:A:398:LEU:HB2	1.95	0.66
1:B:585:ARG:HA	1:B:585:ARG:NE	2.11	0.66
1:B:458:ILE:HD11	1:B:472:MET:SD	2.37	0.65
1:B:536:GLY:HA2	1:B:576:TYR:CE1	2.31	0.65
1:B:30:LYS:HB3	1:B:33:ASP:CG	2.17	0.65
1:B:6:ILE:HA	1:B:28:ARG:O	1.97	0.65
1:A:11:LYS:NZ	1:B:361:GLY:H	1.94	0.65
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.79	0.65
1:B:398:LEU:HD21	1:B:442:PHE:HZ	1.62	0.65
1:A:448:GLY:O	1:A:494:ARG:NH2	2.29	0.64
1:A:182:LEU:H	1:A:182:LEU:CD1	2.09	0.64
1:B:212:ILE:HD12	1:B:212:ILE:N	2.11	0.64
1:A:117:HIS:HB3	1:B:299:GLU:OE2	1.97	0.64
1:A:381:ILE:HD13	1:A:425:PHE:HE1	1.62	0.64
1:A:143:ASN:HD21	1:A:148:ASN:ND2	1.95	0.64
1:A:508:TRP:HB2	1:A:520:VAL:HG23	1.80	0.64
1:B:551:LYS:HE3	1:B:564:GLY:O	1.98	0.64
1:A:331:ASP:HB3	1:B:117:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HG23	1:A:461:ALA:HB1	1.78	0.64
1:A:552:THR:HA	1:A:562:VAL:CB	2.28	0.63
1:A:374:TYR:CZ	1:A:375:LEU:HB2	2.33	0.63
1:B:134:TYR:HB2	1:B:187:VAL:HG11	1.81	0.63
1:A:374:TYR:CG	1:A:375:LEU:N	2.66	0.63
1:B:52:LEU:HD22	1:B:52:LEU:N	2.14	0.63
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.79	0.63
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.63	0.62
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.32	0.62
1:A:134:TYR:CE2	1:A:136:ILE:HD11	2.34	0.62
1:A:386:THR:OG1	1:A:388:GLU:HG2	1.99	0.62
1:A:377:ARG:O	1:A:381:ILE:HG12	1.99	0.62
1:A:251:ALA:O	1:A:255:VAL:HG23	1.99	0.62
1:B:139:GLU:CD	1:B:140:ARG:HH12	2.03	0.62
1:A:18:ILE:HD13	1:A:18:ILE:H	1.63	0.62
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.35	0.62
1:A:2:LEU:HD11	1:B:2:LEU:CD1	2.30	0.62
1:A:376:PHE:CD1	1:A:415:ASN:HB3	2.35	0.61
1:A:1:MET:HE2	1:A:6:ILE:HD11	1.83	0.61
1:B:135:GLN:O	1:B:454:TYR:HB3	2.01	0.61
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.36	0.61
1:A:263:ARG:NH2	1:A:302:GLU:OE1	2.34	0.61
1:B:323:ARG:HD2	1:B:323:ARG:C	2.22	0.60
1:B:135:GLN:HB2	1:B:451:LEU:HD21	1.82	0.60
1:A:4:GLU:OE1	1:B:30:LYS:HE2	2.01	0.60
1:A:191:TYR:CZ	1:A:323:ARG:HG3	2.36	0.60
1:B:224:ARG:HH21	1:B:227:ASP:HB3	1.67	0.60
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.37	0.60
1:A:194:PRO:HD3	1:A:239:ASP:CG	2.22	0.59
1:A:245:ALA:O	1:A:293:MET:HA	2.02	0.59
1:B:356:TRP:CE3	1:B:374:TYR:HB2	2.29	0.59
1:B:256:LEU:HD11	1:B:277:LYS:HG2	1.84	0.59
1:A:330:VAL:HG13	1:A:335:TRP:HE1	1.65	0.59
1:A:458:ILE:HD12	1:A:473:ILE:HB	1.84	0.59
1:A:129:LYS:HD2	1:A:502:ARG:NH1	2.16	0.59
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.37	0.59
1:A:418:ASP:OD2	1:A:418:ASP:N	2.33	0.59
1:A:325:ASN:HA	1:A:354:GLU:OE2	2.01	0.59
1:B:446:TYR:CE1	1:B:505:VAL:HG11	2.36	0.59
1:B:253:ARG:HB3	1:B:253:ARG:NH1	2.17	0.59
1:A:1:MET:HE3	1:A:34:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:CD1	1:A:22:GLN:HB2	2.30	0.59
1:A:63:ASP:OD1	1:A:400:ARG:HD3	2.03	0.58
1:B:350:LEU:HD12	1:B:351:ILE:N	2.17	0.58
1:A:134:TYR:CD2	1:A:136:ILE:HD11	2.37	0.58
1:B:30:LYS:O	1:B:33:ASP:HB2	2.03	0.58
1:A:135:GLN:O	1:A:454:TYR:HB3	2.04	0.58
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.38	0.58
1:B:394:PHE:CZ	1:B:398:LEU:HD11	2.38	0.58
1:B:445:THR:HG21	1:B:580:ILE:HD12	1.85	0.58
1:A:281:THR:HG23	1:A:289:GLN:OE1	2.04	0.58
1:A:304:LYS:HG3	1:A:334:PHE:CD2	2.38	0.58
1:B:523:VAL:HG13	1:B:523:VAL:O	2.04	0.58
1:B:574:ARG:O	1:B:577:GLN:HB2	2.04	0.58
1:B:40:LEU:HD11	1:B:54:HIS:HD1	1.68	0.58
1:B:202:HIS:ND1	1:B:202:HIS:O	2.37	0.58
1:B:328:ASN:HD22	1:B:328:ASN:N	2.01	0.57
1:A:182:LEU:CD1	1:A:182:LEU:N	2.68	0.57
1:B:95:TYR:CE2	1:B:105:ARG:HG3	2.38	0.57
1:A:340:ARG:HH12	1:B:340:ARG:CZ	2.17	0.57
1:A:538:LYS:HB3	1:A:575:PRO:HD3	1.84	0.57
1:B:137:PHE:CE1	1:B:469:ARG:HD3	2.38	0.57
1:A:337:GLU:O	1:A:340:ARG:HB2	2.05	0.57
1:A:224:ARG:HE	1:A:224:ARG:HA	1.68	0.57
1:B:148:ASN:HD22	1:B:149:ASP:N	2.02	0.57
1:B:183:GLU:OE2	1:B:232:ARG:NH1	2.38	0.57
1:A:277:LYS:CD	1:A:277:LYS:H	2.16	0.57
1:A:30:LYS:O	1:A:33:ASP:HB2	2.05	0.57
1:B:522:THR:HG23	1:B:527:HIS:CD2	2.39	0.57
1:A:83:VAL:HG22	1:A:109:GLY:O	2.04	0.57
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.32	0.57
1:A:290:VAL:HG22	1:A:293:MET:HG3	1.85	0.57
1:B:441:LEU:HD23	1:B:441:LEU:C	2.23	0.56
1:B:36:ARG:CG	1:B:36:ARG:HH21	2.15	0.56
1:B:197:ALA:HA	1:B:213:ASP:HA	1.87	0.56
1:B:542:LEU:HD11	1:B:568:GLN:NE2	2.20	0.56
1:A:375:LEU:O	1:A:376:PHE:C	2.41	0.56
1:A:368:PHE:N	1:A:368:PHE:CD2	2.72	0.56
1:A:540:THR:HG22	1:A:572:THR:CG2	2.30	0.56
1:A:178:ARG:HG2	1:A:474:TRP:CZ2	2.41	0.56
1:B:574:ARG:HG2	1:B:577:GLN:OE1	2.06	0.56
1:A:416:LEU:H	1:A:416:LEU:CD2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD13	1:A:484:PHE:CE2	2.40	0.56
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.33	0.56
1:A:143:ASN:HD21	1:A:148:ASN:HD21	1.53	0.56
1:A:194:PRO:HG2	1:A:204:TYR:CD1	2.40	0.56
1:A:389:ILE:CG2	1:A:393:ARG:HG2	2.35	0.56
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.18	0.56
1:B:249:PHE:CE2	1:B:251:ALA:HB3	2.40	0.56
1:B:134:TYR:HB3	1:B:190:LEU:CD1	2.36	0.56
1:B:390:HIS:HA	1:B:515:ASN:OD1	2.06	0.56
1:A:375:LEU:HD23	1:A:401:ALA:HB2	1.88	0.56
1:A:221:THR:O	1:A:224:ARG:HB3	2.05	0.56
1:B:487:TYR:O	1:B:491:ILE:HG12	2.06	0.56
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.70	0.56
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.70	0.56
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.69	0.56
1:A:409:ALA:O	1:A:413:LEU:HD13	2.06	0.55
1:B:359:ALA:O	1:B:363:LEU:HD22	2.06	0.55
1:A:178:ARG:HG2	1:A:474:TRP:CH2	2.41	0.55
1:B:377:ARG:HA	1:B:380:VAL:CG2	2.36	0.55
1:B:492:ARG:O	1:B:496:ARG:HG3	2.05	0.55
1:B:84:PHE:O	1:B:95:TYR:HA	2.06	0.55
1:A:207:ALA:CA	1:A:248:GLN:HG2	2.31	0.55
1:B:442:PHE:HB2	1:B:532:LEU:HD11	1.88	0.55
1:B:377:ARG:HA	1:B:380:VAL:HG22	1.89	0.55
1:B:537:GLU:O	1:B:539:GLN:HG2	2.06	0.55
1:B:286:PHE:CG	1:B:287:ALA:N	2.73	0.55
1:A:341:LEU:O	1:A:344:SER:HB3	2.07	0.55
1:B:561:GLU:C	1:B:563:HIS:H	2.08	0.55
1:B:569:LEU:HD22	1:B:571:LEU:HG	1.88	0.55
1:B:356:TRP:O	1:B:374:TYR:CD2	2.60	0.55
1:A:453:TYR:HB3	1:A:456:ASP:OD2	2.06	0.55
1:B:324:LEU:HD22	1:B:335:TRP:CH2	2.42	0.55
1:A:272:ASP:O	1:A:282:ASN:ND2	2.38	0.54
1:B:185:LEU:HD23	1:B:187:VAL:HG13	1.88	0.54
1:B:39:VAL:HB	1:B:55:ALA:HB3	1.89	0.54
1:A:340:ARG:NH1	1:B:340:ARG:HH12	2.04	0.54
1:A:2:LEU:HD21	1:B:2:LEU:HD13	1.88	0.54
1:B:47:SER:O	1:B:50:GLU:HB3	2.07	0.54
1:B:256:LEU:HD11	1:B:277:LYS:CG	2.38	0.54
1:A:544:GLN:HA	1:A:544:GLN:NE2	2.18	0.54
1:B:376:PHE:O	1:B:380:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:86:LEU:HD13	2.38	0.54
1:A:193:THR:HG22	1:A:194:PRO:CD	2.36	0.54
1:A:380:VAL:HG13	1:A:384:PHE:CD1	2.43	0.54
1:A:44:ARG:NH2	1:A:114:ALA:HA	2.23	0.54
1:B:394:PHE:O	1:B:398:LEU:HD12	2.08	0.54
1:B:326:VAL:O	1:B:326:VAL:HG12	2.08	0.54
1:B:178:ARG:O	1:B:181:TYR:HB3	2.08	0.54
1:B:384:PHE:HE2	1:B:438:LEU:HD22	1.73	0.54
1:A:374:TYR:CD2	1:A:375:LEU:N	2.74	0.54
1:B:135:GLN:HG3	1:B:191:TYR:CE2	2.43	0.54
1:A:30:LYS:HD3	1:A:33:ASP:OD1	2.09	0.53
1:A:504:ASN:ND2	1:A:504:ASN:C	2.62	0.53
1:B:155:GLN:HA	1:B:155:GLN:NE2	2.13	0.53
1:A:193:THR:CG2	1:A:194:PRO:CD	2.85	0.53
1:A:245:ALA:HB2	1:A:296:LEU:HD11	1.90	0.53
1:B:267:TRP:CZ2	1:B:302:GLU:HB3	2.43	0.53
1:B:87:THR:HA	1:B:92:GLU:O	2.08	0.53
1:B:245:ALA:O	1:B:294:PRO:HD2	2.09	0.53
1:B:148:ASN:OD1	1:B:171:ASP:OD2	2.25	0.53
1:A:193:THR:HG23	1:A:194:PRO:HD2	1.90	0.53
1:A:218:ASP:OD2	1:A:220:PRO:HD2	2.09	0.53
1:A:210:LEU:N	1:A:210:LEU:HD12	2.22	0.53
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.43	0.53
1:B:16:TYR:OH	1:B:407:GLU:HG2	2.09	0.53
1:A:277:LYS:HE2	1:A:277:LYS:C	2.28	0.53
1:B:139:GLU:OE2	1:B:167:PHE:HA	2.09	0.52
1:A:467:ASP:O	1:A:470:ARG:HG3	2.10	0.52
1:A:376:PHE:CE1	1:A:415:ASN:HB3	2.45	0.52
1:A:148:ASN:CG	1:A:171:ASP:OD2	2.46	0.52
1:A:44:ARG:HG3	1:A:80:VAL:N	2.24	0.52
1:A:153:THR:HG23	1:A:168:TYR:HA	1.90	0.52
1:B:247:ASP:HB3	1:B:292:ALA:HA	1.90	0.52
1:B:326:VAL:CG1	1:B:329:GLU:HG3	2.38	0.52
1:B:97:GLY:HA3	1:B:108:ALA:O	2.10	0.52
1:A:19:SER:OG	1:A:22:GLN:HG3	2.10	0.52
1:B:250:PHE:CG	1:B:251:ALA:N	2.78	0.52
1:A:59:LYS:HG2	1:A:69:PHE:CE1	2.45	0.52
1:A:350:LEU:HG	1:A:352:VAL:HG23	1.90	0.52
1:A:447:LEU:HB2	1:A:505:VAL:HG23	1.92	0.52
1:B:212:ILE:HD11	1:B:314:TRP:HH2	1.74	0.52
1:B:377:ARG:NH2	1:B:422:THR:HB	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:LEU:HD11	1:B:581:LEU:HD11	1.91	0.51
1:A:44:ARG:HH21	1:A:114:ALA:HA	1.74	0.51
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.42	0.51
1:A:331:ASP:HB3	1:B:117:HIS:HD2	1.76	0.51
1:B:401:ALA:O	1:B:404:LEU:HB2	2.09	0.51
1:B:227:ASP:O	1:B:231:ARG:HG2	2.10	0.51
1:A:489:GLU:O	1:A:493:LEU:HG	2.11	0.51
1:B:440:VAL:O	1:B:444:MET:HG2	2.11	0.51
1:A:11:LYS:HZ2	1:B:361:GLY:H	1.58	0.51
1:B:257:GLN:O	1:B:258:LYS:HD3	2.11	0.51
1:B:545:VAL:HG21	1:B:569:LEU:HB2	1.92	0.51
1:B:488:LYS:CB	1:B:492:ARG:HH11	2.21	0.51
1:A:504:ASN:HD22	1:A:504:ASN:C	2.13	0.51
1:A:219:LEU:HD11	1:A:317:GLN:OE1	2.10	0.51
1:A:523:VAL:HG13	1:A:523:VAL:O	2.11	0.51
1:A:287:ALA:H	1:A:290:VAL:HG11	1.76	0.51
1:B:212:ILE:H	1:B:212:ILE:CD1	2.21	0.51
1:B:404:LEU:HB3	1:B:405:TYR:CD2	2.46	0.51
1:A:88:GLY:HA3	1:A:92:GLU:OE2	2.10	0.51
1:B:44:ARG:HD2	1:B:114:ALA:HA	1.93	0.51
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.92	0.51
1:B:244:HIS:HB3	1:B:295:LYS:HA	1.93	0.51
1:B:373:ASN:HB3	1:B:376:PHE:HB3	1.91	0.51
1:A:494:ARG:HG2	1:A:501:THR:HG22	1.93	0.50
1:B:386:THR:HB	1:B:388:GLU:HG3	1.92	0.50
1:B:536:GLY:CA	1:B:576:TYR:CE1	2.93	0.50
1:A:148:ASN:ND2	1:A:169:GLY:O	2.39	0.50
1:A:178:ARG:O	1:A:182:LEU:HD13	2.11	0.50
1:A:424:ARG:NH2	1:A:454:TYR:O	2.42	0.50
1:B:85:LEU:HD13	1:B:95:TYR:CE2	2.47	0.50
1:B:569:LEU:HD23	1:B:570:LYS:N	2.25	0.50
1:B:243:ASN:ND2	1:B:295:LYS:NZ	2.59	0.50
1:B:253:ARG:CZ	1:B:253:ARG:HB3	2.41	0.50
1:A:269:PHE:HB2	1:A:284:GLU:HB3	1.92	0.50
1:B:582:TRP:CE3	1:B:584:GLY:HA2	2.47	0.50
1:A:304:LYS:HG3	1:A:334:PHE:CE2	2.46	0.50
1:B:40:LEU:HD11	1:B:54:HIS:ND1	2.27	0.50
1:A:133:ILE:HD13	1:A:449:THR:HG21	1.93	0.50
1:A:330:VAL:HG11	1:A:335:TRP:CZ2	2.46	0.50
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.77	0.50
1:B:256:LEU:C	1:B:256:LEU:HD23	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HD3	1:A:70:GLU:HG3	1.93	0.50
1:B:255:VAL:HA	1:B:262:SER:CB	2.42	0.50
1:A:140:ARG:HH12	1:A:201:HIS:HB3	1.77	0.50
1:A:573:LEU:CD2	1:A:579:MET:HG3	2.42	0.49
1:B:133:ILE:HG13	1:B:414:TRP:CE2	2.47	0.49
1:B:175:VAL:CG1	1:B:225:LEU:HD11	2.41	0.49
1:B:455:GLY:N	1:B:457:GLU:OE1	2.46	0.49
1:B:573:LEU:N	1:B:573:LEU:CD2	2.75	0.49
1:B:283:TYR:CD1	1:B:285:THR:HG22	2.48	0.49
1:A:353:GLY:O	1:A:371:VAL:HA	2.11	0.49
1:A:63:ASP:OD2	1:A:63:ASP:C	2.48	0.49
1:B:307:LEU:O	1:B:310:VAL:HB	2.12	0.49
1:B:238:LEU:CD1	1:B:319:ILE:HG21	2.41	0.49
1:B:202:HIS:O	1:B:202:HIS:CG	2.65	0.49
1:B:286:PHE:C	1:B:286:PHE:CD2	2.85	0.49
1:B:64:GLU:H	1:B:396:ALA:HB1	1.78	0.49
1:B:314:TRP:CE3	1:B:314:TRP:HA	2.48	0.49
1:A:263:ARG:O	1:A:263:ARG:HD2	2.13	0.49
1:A:483:LEU:HD21	1:A:487:TYR:CE1	2.47	0.49
1:A:337:GLU:HG2	1:A:340:ARG:HH11	1.77	0.49
1:B:125:PRO:HD3	1:B:369:ASP:OD2	2.13	0.49
1:B:4:GLU:CD	1:B:4:GLU:H	2.16	0.49
1:A:395:ASP:HB2	1:A:517:TYR:CE2	2.48	0.49
1:A:277:LYS:HE2	1:A:277:LYS:N	2.29	0.48
1:B:435:LYS:HG2	1:B:576:TYR:CE2	2.48	0.48
1:A:27:LEU:C	1:A:27:LEU:HD23	2.32	0.48
1:B:485:GLU:OE2	1:B:485:GLU:HA	2.13	0.48
1:A:542:LEU:HD23	1:A:568:GLN:CD	2.34	0.48
1:B:533:ASN:HD22	1:B:573:LEU:HB2	1.77	0.48
1:B:203:LYS:HE3	1:B:216:PHE:CE2	2.48	0.48
1:A:16:TYR:OH	1:A:407:GLU:HG2	2.12	0.48
1:A:562:VAL:O	1:A:562:VAL:CG2	2.54	0.48
1:B:256:LEU:HD21	1:B:277:LYS:HG3	1.95	0.48
1:B:104:GLU:OE1	1:B:107:LYS:NZ	2.38	0.48
1:A:1:MET:HE3	1:A:34:VAL:CG2	2.43	0.48
1:A:105:ARG:O	1:A:105:ARG:HG2	2.13	0.48
1:A:496:ARG:C	1:A:496:ARG:HD3	2.34	0.48
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.42	0.48
1:A:519:PHE:HE2	1:A:521:ARG:HD3	1.79	0.48
1:B:204:TYR:O	1:B:241:VAL:HG11	2.13	0.48
1:B:41:TYR:CE2	1:B:73:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PHE:CZ	1:B:314:TRP:NE1	2.82	0.48
1:B:417:LEU:HD11	1:B:440:VAL:HG12	1.94	0.48
1:B:148:ASN:C	1:B:148:ASN:HD22	2.17	0.48
1:A:516:LEU:HD21	1:A:541:VAL:HG11	1.96	0.48
1:B:504:ASN:C	1:B:504:ASN:HD22	2.16	0.48
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.25	0.48
1:A:122:PHE:HD2	1:A:123:THR:N	2.11	0.48
1:A:355:ILE:HG22	1:A:357:HIS:CD2	2.48	0.48
1:A:137:PHE:CZ	1:A:469:ARG:HD3	2.49	0.48
1:A:4:GLU:HG3	1:B:65:ARG:HB2	1.96	0.48
1:B:245:ALA:HB2	1:B:296:LEU:HD21	1.95	0.48
1:B:411:GLN:HG2	1:B:447:LEU:HD11	1.96	0.47
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.44	0.47
1:B:128:ALA:O	1:B:449:THR:HG21	2.13	0.47
1:B:398:LEU:CD2	1:B:442:PHE:HZ	2.24	0.47
1:B:585:ARG:CA	1:B:585:ARG:NE	2.76	0.47
1:B:330:VAL:HB	1:B:335:TRP:HE1	1.79	0.47
1:A:339:ARG:NH2	1:A:369:ASP:OD1	2.46	0.47
1:A:178:ARG:O	1:A:181:TYR:HB3	2.14	0.47
1:A:528:VAL:HA	1:A:581:LEU:O	2.14	0.47
1:A:540:THR:HA	1:A:572:THR:HA	1.96	0.47
1:A:134:TYR:HB3	1:A:190:LEU:HD23	1.97	0.47
1:A:223:ARG:NH1	1:A:223:ARG:CG	2.77	0.47
1:B:221:THR:O	1:B:224:ARG:HB3	2.14	0.47
1:B:250:PHE:C	1:B:250:PHE:CD1	2.86	0.47
1:B:511:ASP:HB3	1:B:514:ALA:HB3	1.97	0.47
1:A:26:ARG:CG	1:A:70:GLU:HG3	2.43	0.47
1:A:206:THR:C	1:A:248:GLN:HE21	2.18	0.47
1:A:143:ASN:ND2	1:A:148:ASN:HD21	2.13	0.47
1:A:148:ASN:OD1	1:A:215:GLN:O	2.33	0.47
1:B:445:THR:HB	1:B:530:VAL:HG21	1.96	0.47
1:B:530:VAL:HA	1:B:579:MET:O	2.15	0.47
1:B:283:TYR:CE1	1:B:285:THR:HG22	2.49	0.47
1:B:16:TYR:HE1	1:B:18:ILE:HG22	1.79	0.47
1:A:437:ARG:HA	1:A:440:VAL:HG22	1.96	0.47
1:A:458:ILE:HD11	1:A:472:MET:SD	2.55	0.47
1:A:95:TYR:CD2	1:A:105:ARG:HA	2.50	0.47
1:A:286:PHE:CE2	2:A:601:MTT:H262	2.50	0.47
1:B:546:PRO:O	1:B:548:SER:N	2.48	0.47
1:B:36:ARG:HG2	1:B:36:ARG:NH2	2.24	0.47
1:A:148:ASN:ND2	1:A:149:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.30	0.47
1:B:476:GLU:HG2	1:B:477:LYS:N	2.30	0.47
1:B:16:TYR:C	1:B:23:LEU:HD12	2.36	0.46
1:B:85:LEU:HD13	1:B:95:TYR:CZ	2.50	0.46
1:B:8:HIS:CG	1:B:9:GLU:N	2.84	0.46
1:A:416:LEU:O	1:A:416:LEU:HD23	2.15	0.46
1:A:236:ILE:CG2	1:A:238:LEU:HD21	2.45	0.46
1:A:11:LYS:HZ3	1:B:361:GLY:H	1.62	0.46
1:A:313:PHE:O	1:A:316:GLU:HB2	2.14	0.46
1:B:346:ASN:HD22	1:B:349:ALA:HB2	1.80	0.46
1:A:134:TYR:CE2	1:A:136:ILE:CD1	2.99	0.46
1:A:367:GLN:C	1:A:368:PHE:HD2	2.19	0.46
1:B:1:MET:HE1	1:B:86:LEU:HD13	1.98	0.46
1:A:369:ASP:OD1	1:A:369:ASP:N	2.48	0.46
1:A:179:LEU:HB3	1:A:232:ARG:HD2	1.98	0.46
1:A:554:LEU:HD23	1:A:555:ASP:N	2.30	0.46
1:B:134:TYR:HB3	1:B:190:LEU:HD12	1.95	0.46
1:B:182:LEU:O	1:B:187:VAL:HG22	2.16	0.46
1:A:138:PRO:HG3	1:A:195:ILE:HG22	1.97	0.46
1:A:331:ASP:N	1:A:331:ASP:OD1	2.47	0.46
1:A:389:ILE:HG21	1:A:393:ARG:HG2	1.97	0.46
1:B:245:ALA:CB	1:B:296:LEU:HD11	2.45	0.46
1:A:65:ARG:HG2	1:B:4:GLU:HG3	1.96	0.46
1:A:485:GLU:OE2	1:A:488:LYS:HD3	2.15	0.46
1:A:57:ALA:HB1	1:A:70:GLU:C	2.36	0.46
1:A:204:TYR:OH	1:A:323:ARG:NH1	2.48	0.46
1:A:324:LEU:HB2	1:A:327:ALA:HB2	1.98	0.46
1:B:519:PHE:CE1	1:B:530:VAL:HB	2.51	0.46
1:B:256:LEU:HD23	1:B:256:LEU:O	2.16	0.46
1:A:574:ARG:HD2	1:A:577:GLN:HG3	1.98	0.46
1:A:207:ALA:HB2	1:A:248:GLN:HG3	1.98	0.46
1:A:542:LEU:HD23	1:A:568:GLN:NE2	2.31	0.45
1:A:440:VAL:O	1:A:444:MET:HB2	2.16	0.45
1:B:359:ALA:O	1:B:363:LEU:CD2	2.64	0.45
1:A:137:PHE:CE2	1:A:469:ARG:HD3	2.51	0.45
1:B:204:TYR:HB3	1:B:293:MET:CE	2.46	0.45
1:A:134:TYR:HB3	1:A:190:LEU:CD2	2.46	0.45
1:B:315:MET:HA	1:B:319:ILE:HG12	1.97	0.45
1:A:11:LYS:N	1:A:15:ALA:HB3	2.32	0.45
1:A:290:VAL:CG2	1:A:293:MET:HG3	2.46	0.45
1:B:27:LEU:HD23	1:B:27:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.15	0.45
1:B:535:ARG:HB3	1:B:539:GLN:OE1	2.15	0.45
1:B:339:ARG:NH2	1:B:369:ASP:OD1	2.43	0.45
1:A:319:ILE:HD11	1:A:322:TRP:CZ2	2.52	0.45
1:A:405:TYR:CE1	1:A:413:LEU:HD21	2.52	0.45
1:B:538:LYS:HA	1:B:573:LEU:O	2.16	0.45
1:A:290:VAL:O	1:A:290:VAL:HG22	2.16	0.45
1:A:354:GLU:OE1	2:A:601:MTT:H211	2.17	0.45
1:B:245:ALA:HB2	1:B:296:LEU:HD11	1.99	0.45
1:B:24:ARG:NH1	1:B:24:ARG:CG	2.80	0.45
1:A:357:HIS:HA	1:A:374:TYR:CD1	2.52	0.45
1:B:224:ARG:HE	1:B:224:ARG:HA	1.82	0.45
1:A:190:LEU:HG	1:A:234:ILE:CG2	2.47	0.45
1:B:275:VAL:HG12	1:B:282:ASN:CB	2.41	0.45
1:B:52:LEU:HD22	1:B:52:LEU:H	1.81	0.45
1:A:133:ILE:N	1:A:133:ILE:HD12	2.32	0.45
1:A:455:GLY:HA3	1:A:460:MET:HE2	1.99	0.45
1:A:213:ASP:OD2	1:A:214:PRO:HD2	2.17	0.45
1:A:374:TYR:CE2	1:A:375:LEU:HB2	2.52	0.45
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.52	0.45
1:B:143:ASN:ND2	1:B:169:GLY:O	2.49	0.45
1:B:224:ARG:HA	1:B:224:ARG:NE	2.31	0.45
1:B:464:THR:OG1	1:B:465:ASP:N	2.50	0.45
1:B:228:GLU:O	1:B:232:ARG:HD3	2.16	0.44
1:B:465:ASP:HA	1:B:466:PRO:HA	1.70	0.44
1:A:432:ASN:OD1	1:A:434:ALA:HB3	2.16	0.44
1:B:416:LEU:CD2	1:B:416:LEU:N	2.67	0.44
1:A:150:PRO:HB3	1:A:215:GLN:OE1	2.17	0.44
1:B:523:VAL:CG1	1:B:523:VAL:O	2.65	0.44
1:A:416:LEU:HD23	1:A:416:LEU:H	1.82	0.44
1:B:569:LEU:C	1:B:569:LEU:HD23	2.38	0.44
1:A:441:LEU:C	1:A:441:LEU:HD23	2.38	0.44
1:B:26:ARG:CG	1:B:70:GLU:HG3	2.37	0.44
1:B:441:LEU:HD23	1:B:442:PHE:N	2.32	0.44
1:A:336:ARG:O	1:A:340:ARG:HG3	2.16	0.44
1:B:281:THR:CG2	1:B:283:TYR:O	2.65	0.44
1:B:324:LEU:HB2	1:B:353:GLY:HA2	1.99	0.44
1:B:35:VAL:HG22	1:B:87:THR:O	2.17	0.44
1:A:496:ARG:O	1:A:496:ARG:HD3	2.17	0.44
1:B:62:SER:N	1:B:399:THR:HG21	2.32	0.44
1:B:110:VAL:HG13	1:B:110:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:OD1	1:A:79:ARG:NH1	2.50	0.44
1:B:237:ILE:HG23	1:B:321:GLY:C	2.37	0.44
1:A:175:VAL:HG11	1:A:192:PHE:HZ	1.83	0.44
1:B:219:LEU:HD11	1:B:317:GLN:CD	2.38	0.44
1:B:272:ASP:HB2	1:B:282:ASN:ND2	2.32	0.44
1:B:573:LEU:HD11	1:B:579:MET:SD	2.57	0.44
1:A:117:HIS:CE1	1:B:331:ASP:N	2.86	0.44
1:B:48:PRO:C	1:B:50:GLU:H	2.20	0.44
1:B:454:TYR:CD1	1:B:472:MET:HE2	2.53	0.44
1:A:394:PHE:CE2	1:A:398:LEU:HD13	2.53	0.44
1:B:195:ILE:HD13	1:B:195:ILE:H	1.82	0.44
1:B:175:VAL:HG12	1:B:225:LEU:CD1	2.45	0.44
1:A:455:GLY:HA3	1:A:460:MET:CE	2.47	0.44
1:B:389:ILE:HB	1:B:393:ARG:CG	2.47	0.44
1:A:191:TYR:OH	1:A:323:ARG:NE	2.51	0.44
1:A:277:LYS:N	1:A:277:LYS:CD	2.80	0.44
1:B:52:LEU:CD2	1:B:52:LEU:N	2.79	0.44
1:A:422:THR:C	1:A:464:THR:HA	2.38	0.44
1:B:231:ARG:HB2	1:B:231:ARG:HH11	1.83	0.44
1:A:143:ASN:ND2	1:A:148:ASN:ND2	2.63	0.44
1:A:133:ILE:HG22	1:A:451:LEU:HD13	1.99	0.44
1:A:433:GLU:HG2	1:A:437:ARG:HD2	1.99	0.44
1:B:517:TYR:CD2	1:B:518:ALA:N	2.86	0.44
1:B:41:TYR:CD2	1:B:73:LEU:HD12	2.53	0.44
1:A:236:ILE:HG21	1:A:319:ILE:HG22	2.00	0.44
1:B:483:LEU:O	1:B:486:PHE:HB3	2.17	0.44
1:B:341:LEU:HD11	1:B:345:LEU:HD11	1.99	0.44
1:B:154:GLU:OE2	1:B:163:ARG:NH1	2.50	0.44
1:A:83:VAL:HG12	1:A:84:PHE:N	2.31	0.43
1:B:582:TRP:CZ3	1:B:584:GLY:HA2	2.52	0.43
1:A:508:TRP:HZ2	1:A:545:VAL:HG22	1.82	0.43
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.53	0.43
1:B:246:GLY:HA2	1:B:292:ALA:O	2.18	0.43
1:B:346:ASN:HA	1:B:347:PRO:HD2	1.83	0.43
1:B:278:THR:OG1	1:B:279:SER:N	2.50	0.43
1:A:378:GLU:O	1:A:382:ARG:HG3	2.18	0.43
1:A:383:PHE:CD2	1:A:394:PHE:CD1	3.07	0.43
1:A:125:PRO:HD3	1:A:369:ASP:OD2	2.17	0.43
1:A:458:ILE:CG2	1:A:479:GLN:HG2	2.48	0.43
1:A:189:ALA:CB	1:A:235:LYS:HB2	2.47	0.43
1:B:132:VAL:HG11	1:B:491:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:CD2	1:B:105:ARG:HG3	2.53	0.43
1:B:238:LEU:HD12	1:B:319:ILE:HD13	2.01	0.43
1:A:14:TYR:OH	1:A:28:ARG:HD3	2.19	0.43
1:B:377:ARG:NH2	1:B:381:ILE:HD11	2.33	0.43
1:B:63:ASP:HA	1:B:396:ALA:HA	2.01	0.43
1:A:86:LEU:O	1:A:93:ALA:HA	2.17	0.43
1:B:444:MET:HG3	1:B:490:LEU:HB3	2.01	0.43
1:B:375:LEU:HD21	1:B:400:ARG:NH1	2.34	0.43
1:A:426:LEU:HD12	1:A:431:GLY:HA2	2.01	0.43
1:A:193:THR:O	1:A:195:ILE:HG23	2.19	0.43
1:B:44:ARG:HH11	1:B:114:ALA:C	2.22	0.43
1:A:3:LEU:HD13	1:A:101:PHE:CD1	2.54	0.43
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.83	0.43
1:A:415:ASN:HD21	1:A:448:GLY:HA3	1.83	0.43
1:A:190:LEU:HG	1:A:234:ILE:HG21	2.00	0.43
1:A:560:GLU:HG3	1:A:562:VAL:HG13	2.00	0.42
1:B:409:ALA:O	1:B:413:LEU:HG	2.19	0.42
1:B:193:THR:O	1:B:195:ILE:HG23	2.19	0.42
1:A:134:TYR:HE2	1:A:136:ILE:HD11	1.82	0.42
1:B:260:GLU:O	1:B:265:LYS:HD3	2.19	0.42
1:A:7:PHE:CG	1:A:8:HIS:N	2.87	0.42
1:A:203:LYS:HG3	1:A:216:PHE:CE2	2.54	0.42
1:B:332:HIS:CD2	1:B:367:GLN:OE1	2.72	0.42
1:B:219:LEU:N	1:B:220:PRO:CD	2.82	0.42
1:B:223:ARG:HH21	1:B:223:ARG:HG3	1.84	0.42
1:B:398:LEU:HD12	1:B:398:LEU:H	1.85	0.42
1:A:179:LEU:HB2	1:A:180:PRO:HD3	2.02	0.42
1:B:8:HIS:CD2	1:B:84:PHE:HE1	2.38	0.42
1:A:277:LYS:N	1:A:277:LYS:CE	2.83	0.42
1:A:269:PHE:O	1:A:283:TYR:HA	2.18	0.42
1:B:354:GLU:OE1	2:B:701:MTT:H211	2.19	0.42
1:B:1:MET:HE2	1:B:86:LEU:HD13	2.02	0.42
1:A:178:ARG:O	1:A:182:LEU:CD1	2.67	0.42
1:B:203:LYS:NZ	1:B:213:ASP:OD2	2.38	0.42
1:A:523:VAL:CG1	1:A:523:VAL:O	2.67	0.42
1:A:433:GLU:O	1:A:436:PHE:HB3	2.20	0.42
1:B:19:SER:OG	1:B:20:GLU:N	2.53	0.42
1:A:64:GLU:HA	1:A:64:GLU:OE2	2.20	0.42
1:B:411:GLN:HB3	1:B:411:GLN:HE21	1.64	0.42
1:B:337:GLU:O	1:B:340:ARG:HB3	2.19	0.42
1:B:47:SER:HA	1:B:48:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:THR:O	1:A:465:ASP:C	2.56	0.42
1:A:12:GLY:HA2	1:A:364:MET:CE	2.49	0.42
1:A:326:VAL:HG12	1:A:326:VAL:O	2.20	0.42
1:A:200:SER:O	1:A:203:LYS:HE2	2.20	0.42
1:B:423:GLU:HG3	1:B:428:SER:OG	2.20	0.42
1:A:193:THR:HG22	1:A:194:PRO:N	2.35	0.42
1:A:6:ILE:HA	1:A:28:ARG:O	2.20	0.42
1:B:285:THR:O	1:B:286:PHE:C	2.58	0.42
1:A:179:LEU:N	1:A:180:PRO:CD	2.83	0.42
1:B:416:LEU:N	1:B:416:LEU:HD23	2.10	0.41
1:B:383:PHE:HD2	1:B:384:PHE:CE1	2.38	0.41
1:B:454:TYR:HD1	1:B:472:MET:HE2	1.85	0.41
1:A:171:ASP:HB3	1:A:215:GLN:O	2.20	0.41
1:A:411:GLN:OE1	1:A:502:ARG:HA	2.20	0.41
1:A:351:ILE:HB	1:A:369:ASP:OD1	2.20	0.41
1:A:73:LEU:HD12	1:A:73:LEU:N	2.35	0.41
1:A:81:LYS:HA	1:A:111:PHE:O	2.19	0.41
1:A:82:TYR:N	1:A:110:VAL:HG22	2.35	0.41
1:A:554:LEU:C	1:A:554:LEU:HD23	2.40	0.41
1:B:442:PHE:HB2	1:B:532:LEU:CD1	2.51	0.41
1:B:253:ARG:O	1:B:257:GLN:HG3	2.19	0.41
1:B:378:GLU:O	1:B:382:ARG:HG3	2.21	0.41
1:B:553:TRP:CZ3	1:B:583:ASN:HB3	2.55	0.41
1:B:499:SER:HB3	1:B:523:VAL:HG12	2.03	0.41
1:A:297:ARG:HG3	1:A:297:ARG:NH1	2.35	0.41
1:B:134:TYR:OH	1:B:472:MET:HE1	2.21	0.41
1:A:287:ALA:H	1:A:290:VAL:CG1	2.34	0.41
1:A:446:TYR:CD2	1:A:447:LEU:N	2.89	0.41
1:A:1:MET:CE	1:A:34:VAL:HG22	2.49	0.41
1:B:44:ARG:HD3	1:B:114:ALA:O	2.21	0.41
1:B:447:LEU:HD22	1:B:505:VAL:CG2	2.50	0.41
1:A:133:ILE:HD13	1:A:449:THR:CG2	2.50	0.41
1:A:5:ALA:HB1	1:A:66:PHE:HE2	1.86	0.41
1:A:228:GLU:OE2	1:A:231:ARG:NH1	2.53	0.41
1:A:243:ASN:ND2	1:A:244:HIS:HD2	2.19	0.41
1:B:363:LEU:HB3	1:B:409:ALA:HB2	2.03	0.41
1:B:362:TRP:O	1:B:363:LEU:HD13	2.21	0.41
1:A:165:ASP:HA	1:A:201:HIS:CD2	2.54	0.41
1:B:185:LEU:HD23	1:B:187:VAL:CG1	2.49	0.41
1:A:150:PRO:HG3	1:A:167:PHE:CD2	2.56	0.41
1:A:143:ASN:ND2	1:A:169:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:HG11	1:A:573:LEU:HD11	2.03	0.41
1:B:73:LEU:H	1:B:73:LEU:HD22	1.85	0.41
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.56	0.41
1:A:386:THR:CB	1:A:388:GLU:HG2	2.50	0.41
1:B:538:LYS:HB2	1:B:575:PRO:HD3	2.02	0.41
1:B:38:GLU:OE1	1:B:54:HIS:ND1	2.54	0.41
1:A:308:PHE:HB3	1:A:341:LEU:HD22	2.02	0.41
1:B:455:GLY:CA	1:B:457:GLU:OE1	2.68	0.41
1:A:444:MET:HG2	1:A:490:LEU:HB3	2.03	0.41
1:A:420:HIS:HD1	1:A:420:HIS:H	1.69	0.41
1:B:368:PHE:N	1:B:368:PHE:CD1	2.88	0.41
1:A:142:ALA:O	1:A:170:GLY:HA2	2.21	0.41
1:B:3:LEU:CD1	1:B:3:LEU:N	2.84	0.41
1:A:377:ARG:NH1	1:A:381:ILE:CD1	2.76	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.84	0.41
1:A:404:LEU:HB3	1:A:405:TYR:CD2	2.56	0.40
1:B:394:PHE:CD2	1:B:398:LEU:HD11	2.53	0.40
1:B:447:LEU:HB2	1:B:505:VAL:HG22	2.04	0.40
1:B:243:ASN:HD21	1:B:295:LYS:NZ	2.19	0.40
1:B:36:ARG:CG	1:B:36:ARG:NH2	2.76	0.40
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.36	0.40
1:B:134:TYR:HB2	1:B:187:VAL:CG1	2.50	0.40
1:B:500:LEU:HD21	1:B:528:VAL:HG11	2.02	0.40
1:A:27:LEU:HD23	1:A:28:ARG:N	2.35	0.40
1:B:257:GLN:C	1:B:258:LYS:HD3	2.41	0.40
1:B:298:THR:OG1	1:B:330:VAL:HG13	2.21	0.40
1:A:488:LYS:HE2	1:A:492:ARG:HH22	1.87	0.40
1:B:3:LEU:HD12	1:B:3:LEU:N	2.36	0.40
1:A:377:ARG:HH12	1:A:381:ILE:HD11	1.77	0.40
1:B:398:LEU:HD23	1:B:446:TYR:CZ	2.57	0.40
1:A:382:ARG:HA	1:A:386:THR:OG1	2.22	0.40
1:B:528:VAL:HG22	1:B:582:TRP:HD1	1.86	0.40
1:A:238:LEU:HD11	1:A:319:ILE:HG21	2.04	0.40
1:B:363:LEU:N	1:B:363:LEU:HD22	2.36	0.40
1:A:400:ARG:NH1	1:B:99:THR:O	2.54	0.40
1:B:286:PHE:CZ	2:B:701:MTT:H262	2.56	0.40
1:A:436:PHE:CE2	1:A:483:LEU:HD11	2.56	0.40
1:B:122:PHE:CD1	1:B:122:PHE:C	2.95	0.40
1:A:245:ALA:O	1:A:294:PRO:HD2	2.21	0.40
1:A:519:PHE:CE2	1:A:521:ARG:HD3	2.56	0.40
1:A:522:THR:HG23	1:A:526:GLN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	583/585 (100%)	537 (92%)	41 (7%)	5 (1%)	21	60
1	B	583/585 (100%)	534 (92%)	43 (7%)	6 (1%)	19	58
All	All	1166/1170 (100%)	1071 (92%)	84 (7%)	11 (1%)	21	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	GLU
1	B	286	PHE
1	B	547	GLU
1	B	562	VAL
1	B	278	THR
1	A	358	ASP
1	A	547	GLU
1	B	279	SER
1	A	286	PHE
1	A	560	GLU
1	B	288	VAL

5.3.2 Protein sidechains

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	493/493 (100%)	448 (91%)	45 (9%)	12 41
1	B	493/493 (100%)	435 (88%)	58 (12%)	6 27
All	All	986/986 (100%)	883 (90%)	103 (10%)	9 34

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	33	ASP
1	A	35	VAL
1	A	40	LEU
1	A	77	THR
1	A	92	GLU
1	A	112	GLN
1	A	118	ARG
1	A	122	PHE
1	A	143	ASN
1	A	163	ARG
1	A	178	ARG
1	A	180	PRO
1	A	191	TYR
1	A	201	HIS
1	A	214	PRO
1	A	219	LEU
1	A	223	ARG
1	A	224	ARG
1	A	261	GLN
1	A	263	ARG
1	A	277	LYS
1	A	280	ARG
1	A	290	VAL
1	A	293	MET
1	A	330	VAL
1	A	346	ASN
1	A	368	PHE
1	A	369	ASP
1	A	377	ARG
1	A	416	LEU
1	A	418	ASP
1	A	426	LEU
1	A	437	ARG
1	A	454	TYR

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Mol	Chain	Res	Type
1	A	466	PRO
1	A	477	LYS
1	A	496	ARG
1	A	504	ASN
1	A	542	LEU
1	A	544	GLN
1	A	547	GLU
1	A	561	GLU
1	A	563	HIS
1	A	581	LEU
1	B	24	ARG
1	B	25	VAL
1	B	33	ASP
1	B	34	VAL
1	B	36	ARG
1	B	37	CYS
1	B	40	LEU
1	B	65	ARG
1	B	67	ASP
1	B	73	LEU
1	B	75	CYS
1	B	86	LEU
1	B	87	THR
1	B	102	SER
1	B	118	ARG
1	B	122	PHE
1	B	139	GLU
1	B	143	ASN
1	B	148	ASN
1	B	155	GLN
1	B	159	ASP
1	B	164	HIS
1	B	178	ARG
1	B	190	LEU
1	B	195	ILE
1	B	198	SER
1	B	206	THR
1	B	231	ARG
1	B	232	ARG
1	B	250	PHE
1	B	255	VAL
1	B	261	GLN

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Mol	Chain	Res	Type
1	B	296	LEU
1	B	316	GLU
1	B	317	GLN
1	B	323	ARG
1	B	325	ASN
1	B	328	ASN
1	B	344	SER
1	B	382	ARG
1	B	386	THR
1	B	408	GLN
1	B	411	GLN
1	B	416	LEU
1	B	418	ASP
1	B	438	LEU
1	B	451	LEU
1	B	470	ARG
1	B	474	TRP
1	B	483	LEU
1	B	504	ASN
1	B	505	VAL
1	B	522	THR
1	B	535	ARG
1	B	539	GLN
1	B	544	GLN
1	B	573	LEU
1	B	574	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	117	HIS
1	A	135	GLN
1	A	143	ASN
1	A	164	HIS
1	A	215	GLN
1	A	244	HIS
1	A	248	GLN
1	A	325	ASN
1	A	346	ASN
1	A	408	GLN
1	A	411	GLN

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Mol	Chain	Res	Type
1	A	415	ASN
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS
1	A	544	GLN
1	A	566	GLN
1	B	143	ASN
1	B	148	ASN
1	B	155	GLN
1	B	243	ASN
1	B	328	ASN
1	B	332	HIS
1	B	346	ASN
1	B	357	HIS
1	B	367	GLN
1	B	408	GLN
1	B	443	GLN
1	B	495	HIS
1	B	504	ASN
1	B	509	HIS
1	B	513	GLN
1	B	527	HIS
1	B	544	GLN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MTT	A	601	-	48,48,48	0.77	1 (2%)	71,71,71	1.63	8 (11%)
2	MTT	B	701	-	48,48,48	0.76	1 (2%)	71,71,71	1.71	9 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MTT	A	601	-	-	0/20/100/100	0/4/4/4
2	MTT	B	701	-	-	0/20/100/100	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	MTT	O25-C21	2.24	1.47	1.41
2	A	601	MTT	O25-C21	2.41	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	MTT	O43-C43-C42	-2.01	105.81	110.34
2	A	601	MTT	C31-O35-C35	2.00	117.63	113.75
2	A	601	MTT	C31-O44-C44	2.22	123.81	118.01
2	B	701	MTT	O34-C21-C22	2.56	114.34	108.10
2	B	701	MTT	C31-O35-C35	2.82	119.22	113.75
2	A	601	MTT	O45-C41-C42	3.19	114.89	109.80
2	A	601	MTT	C11-O24-C24	3.36	126.80	118.01
2	B	701	MTT	O45-C41-C42	3.41	115.24	109.80
2	A	601	MTT	C42-C43-C44	3.68	117.67	109.60
2	B	701	MTT	C42-C43-C44	3.99	118.37	109.60
2	B	701	MTT	C11-O24-C24	4.03	128.55	118.01
2	B	701	MTT	C21-O34-C34	4.07	128.65	118.01
2	A	601	MTT	C21-O34-C34	5.27	131.78	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	MTT	C41-C42-C43	5.42	118.48	110.43
2	B	701	MTT	C41-C42-C43	5.42	118.49	110.43
2	A	601	MTT	C41-O45-C45	6.48	125.46	113.47
2	B	701	MTT	C41-O45-C45	7.65	127.62	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MTT	2	0
2	B	701	MTT	2	0

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	585/585 (100%)	-0.40	5 (0%) 85 82	9, 30, 53, 72	0
1	B	585/585 (100%)	-0.31	9 (1%) 76 71	11, 32, 59, 88	0
All	All	1170/1170 (100%)	-0.36	14 (1%) 81 76	9, 31, 57, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	SER	4.0
1	A	279	SER	3.9
1	A	274	PRO	3.9
1	B	278	THR	3.0
1	A	563	HIS	2.8
1	B	273	PHE	2.5
1	B	276	SER	2.3
1	B	277	LYS	2.1
1	B	272	ASP	2.1
1	A	278	THR	2.1
1	B	251	ALA	2.1
1	A	272	ASP	2.1
1	B	274	PRO	2.0
1	B	151	PRO	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MTT	B	701	45/45	0.93	0.22	0.63	38,44,50,53	0
2	MTT	A	601	45/45	0.94	0.17	0.08	13,28,42,46	0

6.5 Other polymers

There are no such residues in this entry.