Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:42 PM GMT

PDB ID	:	1GVI
Title	:	THERMUS MALTOGENIC AMYLASE IN COMPLEX WITH BETA-CD
Authors	:	Kim, M.-S.; Kim, J.-I.; Oh, B.-H.
Deposited on	:	2002-02-14
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 (i)) were used in the production of this report:

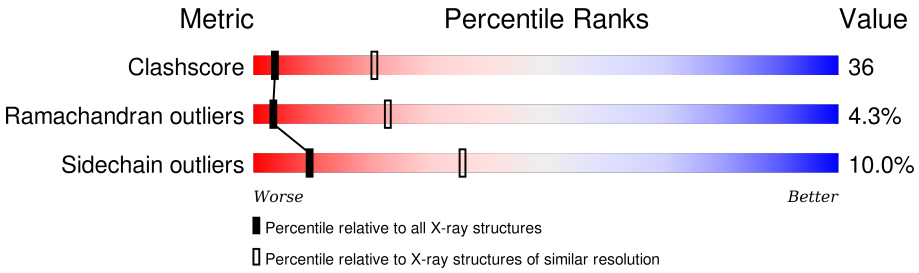
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	588	43% 48% 9%
1	B	588	41% 49% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9810 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.

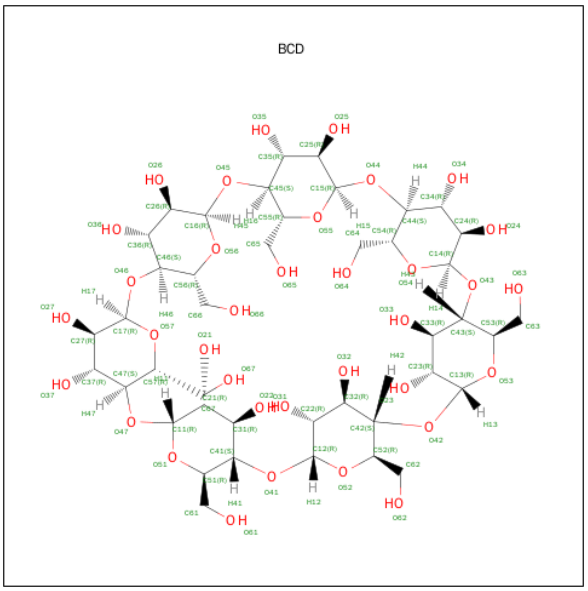
- Molecule 1 is a protein called MALTOGENIC AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4828	3119	819	869	21			
1	B	588	Total	C	N	O	S	0	0	0
			4828	3119	819	869	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	LEU	GLU	CONFLICT	UNP O69007
B	357	LEU	GLU	CONFLICT	UNP O69007

- Molecule 2 is SUGAR (BETA-CYCLODEXTRIN) (three-letter code: BCD) (formula: $C_{42}H_{70}O_{35}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			77	42	35		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	77	42	35	0	0

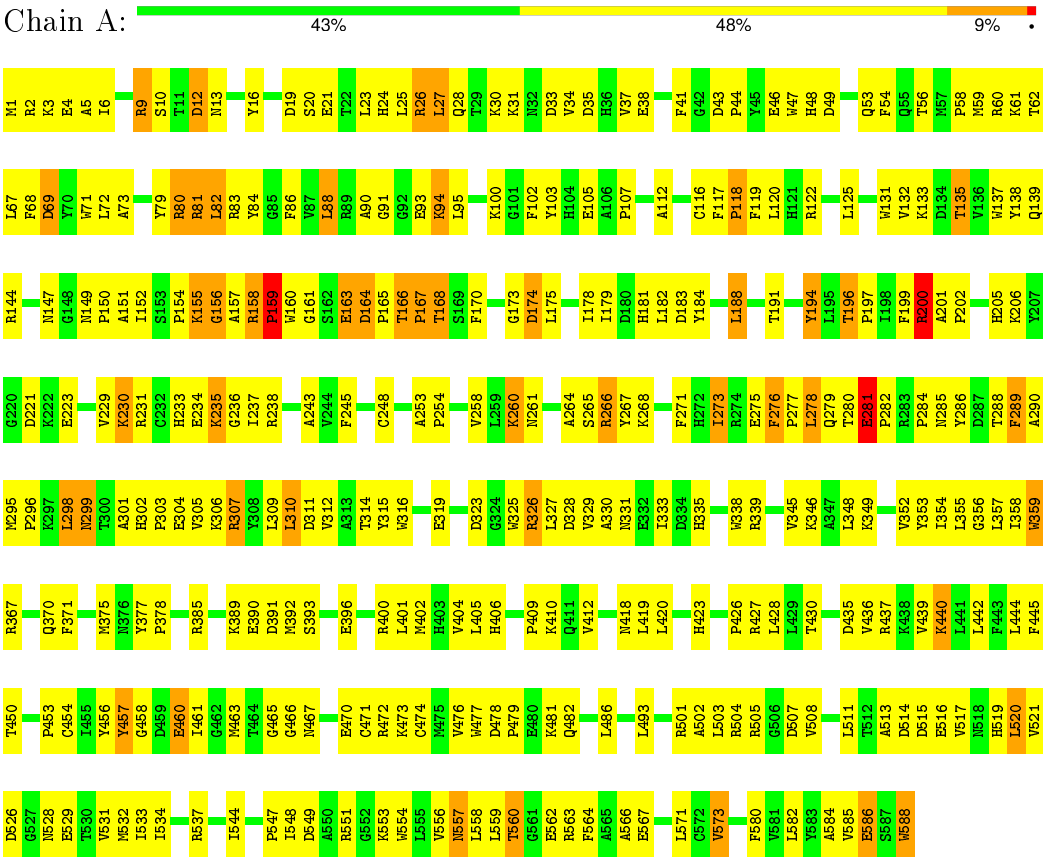
3 Residue-property plots (i)

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.

Note EDS was not executed.

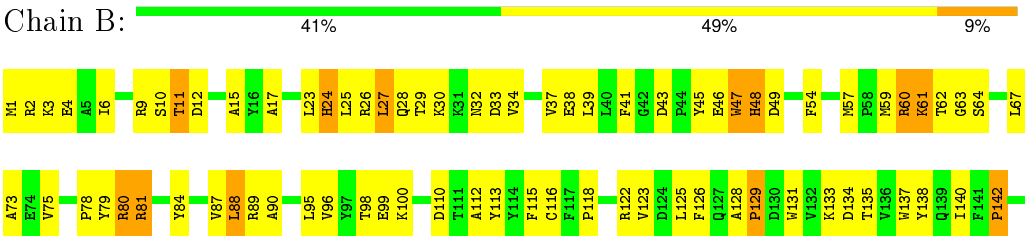
- Molecule 1: MALTOGENIC AMYLASE

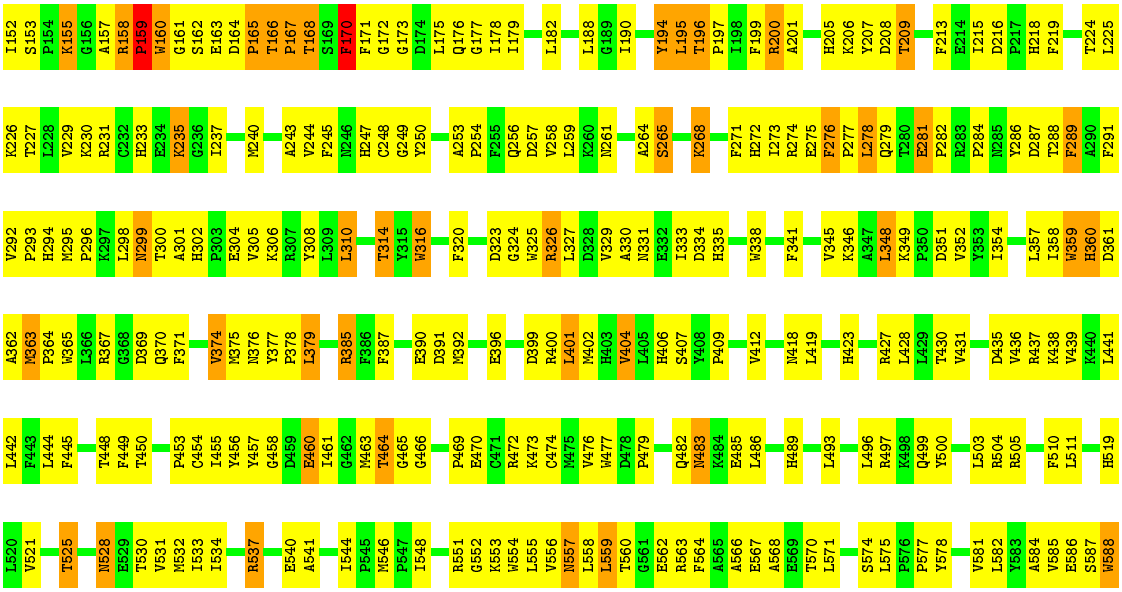
Chain A:



- Molecule 1: MALTOGENIC AMYLASE

Chain B:




I152 S153 P154 K155 G156 A157 R158 P159 W160 G161 S162 E163 D164 P165 T166 P167 T168 S169 F170 F171 G172 G173 D174 L175 Q176 G177 I178 I179 L182 L188 G189 I190 Y194 L195 T196 P197 I198 F199 R200 A201 H205 K206 Y207 D208 T209 F213 E214 I215 D216 P217 H218 F219 T224 L225
K226 T227 L228 V229 K230 R231 C232 H233 E234 K235 G236 I237 M240 A243 V244 F245 N246 H247 C248 G249 Y250 A253 P254 F255 Q256 D257 V258 L259 K260 N261 A264 S265 K268 P271 H272 I273 R274 E275 F276 P277 L278 Q279 T280 E281 P282 R283 P284 N285 Y286 D287 T288 P289 A290 F291
V292 P293 H294 M295 P296 K297 L298 N299 T300 A301 H302 P303 E304 V305 K306 R307 Y308 L309 L310 T314 Y315 W316 F320 D323 G324 W325 R326 L327 D328 V329 A330 N331 E332 I333 D334 H335 W338 F341 V345 K346 A347 L348 K349 P350 D351 V352 Y353 I354 L357 I358 W359 H360 D361
A362 M363 P364 W365 L366 R367 G368 D369 Q370 F371 V374 M375 N376 Y377 P378 L379 R385 F386 F387 E390 D391 M392 E396 D399 R400 L401 M402 H403 V404 L405 H406 S407 Y408 P409 V412 M418 L419 H423 R427 L428 L429 T430 V431 D435 V436 R437 K438 V439 K440 L441
L442 F443 L444 F445 T448 F449 T450 P453 C454 I455 Y456 Y457 G458 D459 E460 I461 G462 M463 T464 G465 G466 P469 E470 C471 R472 K473 C474 M475 V476 W477 D478 P479 Q482 N483 K484 E485 L486 H489 L493 L496 R497 K498 Q499 Y500 L503 R504 R505 F510 L511 H519
L520 V521 T525 N528 E529 T530 V531 M532 I533 I534 R537 E540 A541 I544 P545 M546 P547 I548 R551 G552 K553 W554 L555 V556 N557 L558 L559 T560 G561 E562 R563 F564 A565 A566 E567 A568 E569 T570 L571 S574 L575 P576 P577 Y578 V581 L582 Y583 A584 V585 E586 S587 W588

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	119.09Å 119.09Å 270.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	89.3 (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0/4982	0.67	0/6770
1	B	0.42	0/4982	0.68	1/6770 (0.0%)
All	All	0.41	0/9964	0.68	1/13540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	PHE	N-CA-C	6.04	127.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4828	0	4629	347	0
1	B	4828	0	4629	349	0
2	A	77	0	70	2	0
2	B	77	0	70	3	0
All	All	9810	0	9398	683	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 36.

All (683) 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:281:GLU:HB2	1:A:282:PRO:HD3	1.33	1.08
1:B:281:GLU:HB2	1:B:282:PRO:CD	1.93	0.99
1:B:275:GLU:HG3	1:B:277:PRO:HD2	1.46	0.97
1:B:155:LYS:HG3	1:B:170:PHE:HB2	1.47	0.96
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.44	0.95
1:A:357:LEU:HD22	1:A:375:MET:HG3	1.50	0.93
1:B:29:THR:HG1	1:B:71:TRP:HZ3	1.00	0.93
1:B:558:LEU:HD11	1:B:584:ALA:HB2	1.49	0.92
1:A:31:LYS:HA	1:A:69:ASP:OD1	1.70	0.91
1:A:44:PRO:HD3	1:A:82:LEU:HA	1.53	0.90
1:A:281:GLU:HB2	1:A:282:PRO:CD	2.02	0.89
1:B:281:GLU:HB2	1:B:282:PRO:HD3	1.52	0.88
1:A:160:TRP:HB3	1:A:165:PRO:HB3	1.55	0.88
1:A:158:ARG:HB3	1:A:159:PRO:HD2	1.56	0.87
1:B:253:ALA:HB3	1:B:254:PRO:HD3	1.54	0.87
1:B:133:LYS:HB2	1:B:505:ARG:HH21	1.39	0.87
1:B:557:ASN:HD21	1:B:559:LEU:HD12	1.36	0.87
1:B:64:SER:HB2	1:B:68:PHE:O	1.77	0.85
1:B:430:THR:HG21	1:B:465:GLY:H	1.39	0.85
1:B:333:ILE:HD12	1:B:338:TRP:CZ2	2.12	0.84
1:A:88:LEU:HD23	1:A:88:LEU:N	1.93	0.83
1:A:513:ALA:HB3	1:A:516:GLU:HG2	1.59	0.82
1:B:88:LEU:H	1:B:88:LEU:HD23	1.44	0.82
1:B:291:PHE:O	1:B:293:PRO:HD3	1.80	0.81
1:B:164:ASP:HB2	1:B:165:PRO:HD3	1.63	0.80
1:A:557:ASN:HB3	1:A:560:THR:HG22	1.64	0.80
1:B:87:VAL:HG22	1:B:96:VAL:HG22	1.63	0.80
1:A:401:LEU:HD21	1:A:445:PHE:HZ	1.46	0.80
1:B:556:VAL:HG13	1:B:584:ALA:HB3	1.61	0.79
1:A:554:TRP:H	1:A:586:GLU:HB2	1.46	0.79
1:A:81:ARG:HB2	1:A:118:PRO:O	1.81	0.79
1:B:314:THR:HG22	1:B:348:LEU:HD12	1.63	0.79
1:A:275:GLU:HB3	1:A:285:ASN:HD22	1.48	0.79
1:A:400:ARG:NH2	1:B:100:LYS:HD3	1.98	0.78
1:B:430:THR:CG2	1:B:465:GLY:H	1.96	0.78
1:A:167:PRO:HG2	1:A:168:THR:H	1.49	0.78
1:A:553:LYS:HE3	1:A:554:TRP:NE1	1.98	0.78
1:A:419:LEU:HD23	1:A:419:LEU:H	1.50	0.77
1:A:149:ASN:ND2	1:A:151:ALA:HB2	1.99	0.76
1:A:158:ARG:CB	1:A:159:PRO:HD2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HG2	1:A:73:ALA:HB2	1.69	0.75
1:A:291:PHE:O	1:A:293:PRO:HD3	1.87	0.75
1:A:557:ASN:ND2	1:A:559:LEU:H	1.84	0.74
1:B:326:ARG:HD2	1:B:326:ARG:C	2.08	0.74
1:B:261:ASN:HB3	1:B:264:ALA:HB3	1.69	0.74
1:A:30:LYS:HB3	1:A:33:ASP:HB2	1.68	0.74
1:A:243:ALA:HB2	1:A:325:TRP:CE3	2.23	0.74
1:B:345:VAL:HG23	1:B:346:LYS:H	1.53	0.73
1:A:158:ARG:HD3	1:A:159:PRO:HD2	1.70	0.73
1:A:266:ARG:HE	1:A:266:ARG:HA	1.53	0.73
1:B:357:LEU:CD2	1:B:375:MET:HG3	2.19	0.73
1:B:6:ILE:HD13	1:B:88:LEU:HD11	1.70	0.73
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.54	0.73
1:A:359:TRP:CZ3	1:B:112:ALA:HB2	2.23	0.73
1:A:59:MET:HE1	1:A:86:PHE:HD2	1.52	0.73
1:A:461:ILE:HB	1:A:482:GLN:HB2	1.70	0.73
1:B:450:THR:HG23	1:B:505:ARG:HA	1.72	0.72
1:B:39:LEU:HD12	1:B:57:MET:HE2	1.70	0.72
1:B:557:ASN:ND2	1:B:559:LEU:H	1.87	0.72
1:A:158:ARG:CD	1:A:159:PRO:HD2	2.20	0.72
1:B:400:ARG:O	1:B:404:VAL:HG12	1.89	0.72
1:B:461:ILE:HB	1:B:482:GLN:HB2	1.69	0.72
1:A:88:LEU:HD23	1:A:88:LEU:H	1.53	0.72
1:A:520:LEU:HD12	1:A:521:VAL:N	2.04	0.71
1:A:34:VAL:HG13	1:A:90:ALA:HB2	1.72	0.71
1:A:167:PRO:CG	1:A:168:THR:H	2.02	0.71
1:A:560:THR:HG23	1:A:562:GLU:H	1.55	0.71
1:A:448:THR:OG1	1:A:503:LEU:HD22	1.90	0.71
1:A:3:LYS:HE2	1:A:95:LEU:HD21	1.72	0.71
1:A:158:ARG:HD3	1:A:159:PRO:CD	2.20	0.71
1:A:102:PHE:C	1:A:103:TYR:HD1	1.94	0.71
1:B:196:THR:HG23	1:B:197:PRO:CD	2.21	0.71
1:A:175:LEU:HD13	1:A:219:PHE:HB3	1.70	0.71
1:B:554:TRP:HB2	1:B:586:GLU:HB3	1.73	0.70
1:A:260:LYS:HE3	1:A:260:LYS:HA	1.72	0.70
1:A:160:TRP:HB3	1:A:165:PRO:CB	2.20	0.70
1:A:112:ALA:HB2	1:B:359:TRP:CZ3	2.25	0.70
1:B:345:VAL:HG23	1:B:346:LYS:N	2.07	0.70
1:B:330:ALA:HB1	1:B:371:PHE:CZ	2.27	0.69
1:B:88:LEU:N	1:B:88:LEU:HD23	2.07	0.69
1:A:401:LEU:HD21	1:A:445:PHE:CZ	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:C	1:A:165:PRO:HD3	2.13	0.69
1:B:281:GLU:CB	1:B:282:PRO:HD3	2.22	0.69
1:B:196:THR:HG23	1:B:197:PRO:HD2	1.74	0.69
1:A:132:VAL:HG11	1:A:353:TYR:CD1	2.27	0.69
1:A:359:TRP:HZ3	1:B:112:ALA:HB2	1.56	0.68
1:B:385:ARG:HH11	1:B:392:MET:HE3	1.58	0.68
1:A:271:PHE:HB2	1:A:273:ILE:HD11	1.75	0.68
1:A:532:MET:C	1:A:533:ILE:HD12	2.13	0.68
1:A:534:ILE:HD13	1:A:573:VAL:HG11	1.76	0.68
1:B:357:LEU:HD22	1:B:375:MET:HG3	1.76	0.68
1:B:230:LYS:O	1:B:230:LYS:HD3	1.93	0.68
1:A:64:SER:HB2	1:A:68:PHE:O	1.93	0.68
1:B:423:HIS:HB2	1:B:472:ARG:HE	1.58	0.68
1:A:333:ILE:HD12	1:A:338:TRP:CZ2	2.29	0.68
1:B:548:ILE:HD11	1:B:568:ALA:O	1.93	0.67
1:B:326:ARG:HD2	1:B:326:ARG:O	1.93	0.67
1:B:63:GLY:HA3	1:B:402:MET:CE	2.25	0.67
1:A:430:THR:CG2	1:A:465:GLY:H	2.08	0.67
1:B:511:LEU:HD12	1:B:511:LEU:N	2.09	0.67
1:B:79:TYR:O	1:B:81:ARG:HD3	1.95	0.67
1:A:112:ALA:HB2	1:B:359:TRP:HZ3	1.58	0.66
1:A:520:LEU:HD11	1:A:522:TYR:HD1	1.60	0.66
1:A:409:PRO:HG2	1:A:412:VAL:HG23	1.78	0.66
1:B:155:LYS:HE3	1:B:170:PHE:HB3	1.77	0.66
1:B:387:PHE:HB2	1:B:442:LEU:HD21	1.78	0.66
1:B:159:PRO:C	1:B:165:PRO:HG2	2.16	0.66
1:A:44:PRO:HD2	1:A:81:ARG:HG2	1.77	0.65
1:A:12:ASP:HB3	1:A:363:MET:SD	2.36	0.65
1:B:281:GLU:CB	1:B:282:PRO:CD	2.73	0.65
1:A:142:PRO:HD2	1:A:196:THR:HG22	1.77	0.65
1:A:436:VAL:CG1	1:A:486:LEU:HD13	2.27	0.65
1:A:31:LYS:HG3	1:A:67:LEU:O	1.97	0.65
1:A:273:ILE:HD12	1:A:273:ILE:N	2.12	0.65
1:A:116:CYS:HB3	1:B:360:HIS:CD2	2.31	0.65
1:A:557:ASN:C	1:A:557:ASN:HD22	2.00	0.65
1:A:160:TRP:CB	1:A:165:PRO:HB3	2.27	0.65
1:A:400:ARG:HH21	1:B:100:LYS:HD3	1.60	0.65
1:A:558:LEU:HD11	1:A:584:ALA:HB2	1.77	0.64
1:B:226:LYS:O	1:B:230:LYS:HB2	1.96	0.64
1:B:537:ARG:HH11	1:B:537:ARG:HB3	1.62	0.64
1:B:553:LYS:HB2	1:B:588:TRP:CE3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HA	1:B:71:TRP:O	1.97	0.64
1:A:377:TYR:N	1:A:378:PRO:HD2	2.13	0.64
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.61	0.64
1:A:221:ASP:OD2	1:A:223:GLU:HB2	1.98	0.64
1:A:284:PRO:HG3	1:A:293:PRO:HG3	1.79	0.64
1:B:137:TRP:O	1:B:454:CYS:HA	1.97	0.64
1:B:392:MET:HB2	1:B:396:GLU:HB2	1.80	0.64
1:A:302:HIS:CG	1:A:303:PRO:HD2	2.33	0.64
1:A:155:LYS:HG3	1:A:156:GLY:H	1.63	0.64
1:B:166:THR:HG21	1:B:469:PRO:O	1.98	0.64
1:B:3:LYS:HE2	1:B:95:LEU:HD21	1.79	0.64
1:A:253:ALA:HB3	1:A:254:PRO:CD	2.24	0.63
1:A:544:ILE:O	1:A:573:VAL:HG12	1.98	0.63
1:B:64:SER:HB3	1:B:69:ASP:HA	1.80	0.63
1:A:357:LEU:CD2	1:A:375:MET:HG3	2.25	0.63
1:A:100:LYS:HD3	1:B:400:ARG:NH2	2.13	0.63
1:B:556:VAL:CG1	1:B:584:ALA:HB3	2.29	0.63
1:B:532:MET:C	1:B:533:ILE:HD12	2.18	0.63
1:A:253:ALA:CB	1:A:254:PRO:HD3	2.26	0.63
1:B:284:PRO:HB3	1:B:286:TYR:CE1	2.34	0.63
1:B:385:ARG:HD3	1:B:391:ASP:OD2	1.98	0.63
1:B:357:LEU:HD23	1:B:375:MET:HE2	1.80	0.62
1:A:345:VAL:HG23	1:A:346:LYS:N	2.14	0.62
1:B:461:ILE:CD1	1:B:463:MET:HG3	2.30	0.62
1:B:533:ILE:HD12	1:B:533:ILE:N	2.14	0.62
1:A:503:LEU:HD21	1:A:531:VAL:HG11	1.80	0.62
1:A:439:VAL:HG11	1:A:486:LEU:HD21	1.81	0.62
1:A:436:VAL:HG13	1:A:486:LEU:HD13	1.82	0.62
1:A:548:ILE:HD11	1:A:571:LEU:HB2	1.82	0.62
1:A:553:LYS:HE3	1:A:554:TRP:HE1	1.64	0.62
1:B:265:SER:O	1:B:268:LYS:HD3	1.99	0.62
1:A:360:HIS:CD2	1:B:116:CYS:HB3	2.34	0.62
1:B:450:THR:HG23	1:B:504:ARG:O	2.00	0.61
1:B:553:LYS:H	1:B:587:SER:HA	1.65	0.61
1:A:427:ARG:HH12	1:A:458:GLY:H	1.49	0.61
1:A:450:THR:HG23	1:A:504:ARG:O	2.00	0.61
1:B:62:THR:OG1	1:B:406:HIS:HE1	1.83	0.61
1:A:165:PRO:O	1:A:166:THR:CB	2.48	0.61
1:A:167:PRO:O	1:A:168:THR:OG1	2.19	0.61
1:A:423:HIS:CD2	1:A:423:HIS:H	2.17	0.61
1:B:152:ILE:HB	1:B:155:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HB3	1:B:159:PRO:HD2	1.81	0.61
1:B:179:ILE:HA	1:B:182:LEU:HD13	1.82	0.61
1:A:60:ARG:HH12	1:A:72:LEU:HD23	1.64	0.61
1:B:444:LEU:HA	1:B:493:LEU:HD21	1.83	0.61
1:A:238:ARG:HD2	1:A:323:ASP:CG	2.21	0.60
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.16	0.60
1:B:449:PHE:O	1:B:497:ARG:NH2	2.35	0.60
1:A:133:LYS:HB2	1:A:505:ARG:HH21	1.67	0.60
1:A:444:LEU:HA	1:A:493:LEU:HD21	1.84	0.60
1:B:525:THR:HG23	1:B:530:THR:HG23	1.83	0.60
1:B:444:LEU:HD11	1:B:582:LEU:HD11	1.83	0.60
1:A:439:VAL:HG12	1:A:486:LEU:HD11	1.83	0.60
1:A:149:ASN:HD21	1:A:151:ALA:HB2	1.66	0.59
1:A:277:PRO:O	1:A:279:GLN:HG3	2.02	0.59
1:A:248:CYS:O	1:A:296:PRO:HD2	2.01	0.59
1:B:39:LEU:HD12	1:B:57:MET:CE	2.32	0.59
1:A:358:ILE:HG23	1:A:360:HIS:CE1	2.38	0.59
1:A:278:LEU:HA	1:A:285:ASN:HD21	1.67	0.59
1:B:419:LEU:H	1:B:419:LEU:HD23	1.67	0.59
1:A:449:PHE:CE1	1:A:508:VAL:HG11	2.38	0.59
1:A:349:LYS:HB3	1:A:352:VAL:HG23	1.84	0.59
1:B:560:THR:HG22	1:B:562:GLU:H	1.65	0.59
1:B:229:VAL:HG11	1:B:320:PHE:O	2.01	0.59
1:B:197:PRO:O	1:B:206:LYS:HB2	2.03	0.59
1:A:557:ASN:HD22	1:A:559:LEU:H	1.50	0.58
1:A:175:LEU:CD1	1:A:219:PHE:HB3	2.32	0.58
1:A:79:TYR:O	1:A:81:ARG:HD2	2.02	0.58
1:B:175:LEU:HD13	1:B:219:PHE:HB3	1.85	0.58
1:A:140:ILE:O	1:A:140:ILE:HG13	2.04	0.58
1:B:131:TRP:O	1:B:135:THR:HG23	2.04	0.58
1:B:160:TRP:HB3	1:B:165:PRO:HD3	1.85	0.58
1:B:250:TYR:HB2	1:B:294:HIS:HB2	1.86	0.58
1:A:402:MET:HE3	1:A:406:HIS:CD2	2.39	0.58
1:B:161:GLY:HA3	1:B:164:ASP:OD2	2.03	0.58
1:A:144:ARG:HG3	1:A:472:ARG:O	2.04	0.58
1:A:254:PRO:O	1:A:258:VAL:HG23	2.03	0.58
1:B:10:SER:O	1:B:11:THR:HB	2.03	0.58
1:A:94:LYS:HD2	1:A:94:LYS:C	2.24	0.58
1:B:557:ASN:ND2	1:B:559:LEU:N	2.52	0.58
1:B:64:SER:CB	1:B:69:ASP:HA	2.34	0.58
1:B:155:LYS:HZ1	1:B:172:GLY:HA2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:O	1:A:155:LYS:HB2	2.02	0.57
1:B:190:ILE:HD12	1:B:190:ILE:C	2.25	0.57
1:B:6:ILE:HA	1:B:28:GLN:O	2.03	0.57
1:B:197:PRO:HB2	1:B:206:LYS:HB3	1.87	0.57
1:A:12:ASP:OD1	1:A:367:ARG:NH1	2.37	0.57
1:B:470:GLU:O	1:B:473:LYS:HG3	2.05	0.57
1:A:513:ALA:C	1:A:515:ASP:H	2.08	0.57
1:B:273:ILE:N	1:B:273:ILE:HD12	2.19	0.57
1:B:458:GLY:N	1:B:460:GLU:OE2	2.37	0.57
1:B:302:HIS:CD2	1:B:304:GLU:H	2.23	0.57
1:B:358:ILE:HB	1:B:374:VAL:HG11	1.87	0.57
1:A:231:ARG:O	1:A:235:LYS:HD3	2.05	0.57
1:A:196:THR:OG1	1:A:197:PRO:HD2	2.05	0.57
1:B:292:VAL:O	1:B:292:VAL:HG12	2.04	0.57
1:A:88:LEU:N	1:A:88:LEU:CD2	2.67	0.57
1:A:331:ASN:HB3	1:A:358:ILE:HG12	1.86	0.57
1:A:557:ASN:CB	1:A:560:THR:HG22	2.34	0.56
1:B:160:TRP:HB3	1:B:165:PRO:CG	2.35	0.56
1:A:409:PRO:HG2	1:A:412:VAL:CG2	2.35	0.56
1:B:349:LYS:O	1:B:352:VAL:HG23	2.05	0.56
1:B:205:HIS:CD2	2:B:1589:BCD:H25	2.39	0.56
1:B:333:ILE:HD12	1:B:338:TRP:HZ2	1.68	0.56
1:B:243:ALA:HB2	1:B:325:TRP:CE3	2.40	0.56
1:A:511:LEU:N	1:A:511:LEU:HD12	2.20	0.56
1:B:461:ILE:HD11	1:B:463:MET:HG3	1.88	0.56
1:B:17:ALA:HA	1:B:23:LEU:HD23	1.87	0.56
1:A:315:TYR:CE1	1:A:319:GLU:HG3	2.41	0.56
1:A:284:PRO:CG	1:A:293:PRO:HG3	2.35	0.56
1:B:567:GLU:O	1:B:568:ALA:HB2	2.06	0.56
1:A:19:ASP:OD1	1:A:21:GLU:N	2.38	0.56
1:A:588:TRP:C	1:A:588:TRP:CE3	2.78	0.56
1:A:393:SER:HB2	1:A:517:VAL:HG13	1.88	0.56
1:B:165:PRO:HB3	1:B:171:PHE:HZ	1.71	0.56
1:B:537:ARG:NH1	1:B:537:ARG:HB3	2.21	0.56
1:A:6:ILE:HD13	1:A:88:LEU:HD11	1.87	0.56
1:B:188:LEU:HD23	1:B:188:LEU:O	2.05	0.56
1:B:557:ASN:C	1:B:557:ASN:HD22	2.09	0.55
1:A:330:ALA:HB1	1:A:371:PHE:CZ	2.41	0.55
1:A:553:LYS:HB3	1:A:586:GLU:HB3	1.87	0.55
1:A:167:PRO:CG	1:A:168:THR:N	2.69	0.55
1:A:230:LYS:O	1:A:234:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HA	1:A:71:TRP:O	2.07	0.55
1:B:548:ILE:O	1:B:548:ILE:HG13	2.05	0.55
1:B:521:VAL:HG23	1:B:534:ILE:HD13	1.88	0.55
1:B:390:GLU:OE2	1:B:438:LYS:HE2	2.07	0.55
1:B:259:LEU:HD23	1:B:278:LEU:HD23	1.89	0.55
1:A:516:GLU:HB2	1:A:519:HIS:HB2	1.89	0.55
1:B:27:LEU:HD12	1:B:37:VAL:HG21	1.89	0.55
1:A:24:HIS:C	1:A:25:LEU:HD22	2.26	0.55
1:B:152:ILE:HB	1:B:155:LYS:HZ3	1.72	0.55
1:B:377:TYR:N	1:B:378:PRO:HD2	2.21	0.54
1:A:157:ALA:O	1:A:158:ARG:O	2.26	0.54
1:B:476:VAL:O	1:B:482:GLN:NE2	2.40	0.54
1:A:23:LEU:HG	1:A:120:LEU:HD12	1.90	0.54
1:B:131:TRP:HE1	1:B:351:ASP:HB3	1.73	0.54
1:B:331:ASN:HB3	1:B:358:ILE:HG12	1.89	0.54
1:A:237:ILE:HD12	1:A:237:ILE:N	2.23	0.54
1:A:470:GLU:O	1:A:473:LYS:HG3	2.07	0.54
1:B:155:LYS:HE3	1:B:170:PHE:CB	2.37	0.54
1:A:520:LEU:C	1:A:520:LEU:HD12	2.27	0.54
1:B:168:THR:HG22	1:B:168:THR:O	2.07	0.54
1:A:563:ARG:O	1:A:563:ARG:HD2	2.07	0.54
1:A:430:THR:HG21	1:A:465:GLY:H	1.72	0.54
1:A:456:TYR:O	1:A:458:GLY:N	2.41	0.54
1:B:167:PRO:CD	1:B:168:THR:H	2.21	0.54
1:A:554:TRP:H	1:A:586:GLU:CB	2.17	0.54
1:B:288:THR:O	1:B:289:PHE:C	2.46	0.54
1:A:236:GLY:C	1:A:237:ILE:HD12	2.28	0.54
1:B:357:LEU:HD23	1:B:375:MET:HG3	1.88	0.54
1:A:34:VAL:HG11	1:A:88:LEU:HB2	1.89	0.54
1:A:10:SER:HB3	1:A:84:TYR:OH	2.08	0.54
1:B:208:ASP:O	1:B:249:GLY:HA3	2.07	0.54
1:A:140:ILE:HD12	1:A:178:ILE:HG12	1.90	0.53
1:A:292:VAL:HG12	1:A:292:VAL:O	2.08	0.53
1:B:155:LYS:CG	1:B:170:PHE:HB2	2.30	0.53
1:A:80:ARG:HD2	1:A:119:PHE:CE2	2.43	0.53
1:A:537:ARG:O	1:A:537:ARG:HD2	2.08	0.53
1:B:254:PRO:O	1:B:258:VAL:HG23	2.09	0.53
1:A:559:LEU:HD11	1:A:580:PHE:HE1	1.72	0.53
1:B:230:LYS:C	1:B:230:LYS:HD3	2.29	0.53
1:B:329:VAL:O	1:B:329:VAL:HG12	2.08	0.53
1:B:306:LYS:O	1:B:310:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASN:O	1:A:470:GLU:HB2	2.09	0.53
1:A:137:TRP:HB2	1:A:454:CYS:HB2	1.91	0.53
1:B:418:ASN:O	1:B:453:PRO:HA	2.09	0.53
1:A:553:LYS:HD2	1:A:588:TRP:HB3	1.91	0.53
1:A:385:ARG:HG2	1:A:391:ASP:HB2	1.91	0.53
1:A:64:SER:HB3	1:A:69:ASP:HA	1.90	0.53
1:B:466:GLY:O	1:B:470:GLU:HB2	2.09	0.52
1:B:98:THR:HB	1:B:113:TYR:O	2.09	0.52
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.74	0.52
1:A:428:LEU:HD11	1:A:442:LEU:HD13	1.91	0.52
1:A:158:ARG:HD3	1:A:159:PRO:HD3	1.91	0.52
1:A:1:MET:HE2	1:A:95:LEU:HD22	1.91	0.52
1:B:131:TRP:O	1:B:134:ASP:N	2.41	0.52
1:B:26:ARG:HG3	1:B:26:ARG:NH1	2.25	0.52
1:A:167:PRO:HG2	1:A:168:THR:N	2.22	0.52
1:A:393:SER:OG	1:A:396:GLU:HG3	2.10	0.52
1:A:206:LYS:HE2	1:A:219:PHE:CE1	2.44	0.52
1:B:430:THR:HG21	1:B:465:GLY:N	2.18	0.52
1:A:254:PRO:HB3	1:A:267:TYR:CD2	2.45	0.52
1:B:201:ALA:HB3	1:B:206:LYS:HG3	1.92	0.52
1:B:60:ARG:NH1	1:B:72:LEU:HD23	2.25	0.52
1:A:173:GLY:O	1:A:174:ASP:HB3	2.09	0.52
1:B:557:ASN:HD22	1:B:559:LEU:N	2.08	0.51
1:B:557:ASN:HD22	1:B:558:LEU:N	2.08	0.51
1:B:345:VAL:CG2	1:B:346:LYS:H	2.21	0.51
1:B:552:GLY:HA2	1:B:587:SER:HB3	1.92	0.51
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.75	0.51
1:A:516:GLU:CB	1:A:519:HIS:HB2	2.40	0.51
1:A:385:ARG:HB3	1:A:392:MET:CE	2.41	0.51
1:B:155:LYS:HG3	1:B:170:PHE:CB	2.30	0.51
1:A:588:TRP:OXT	1:A:588:TRP:CD2	2.63	0.51
1:B:199:PHE:O	1:B:200:ARG:C	2.49	0.51
1:B:362:ALA:CB	1:B:374:VAL:HG21	2.41	0.51
1:B:247:HIS:HA	1:B:298:LEU:HD13	1.91	0.51
1:A:260:LYS:HE3	1:A:260:LYS:CA	2.41	0.51
1:A:41:PHE:O	1:A:54:PHE:HB2	2.11	0.51
1:B:240:MET:HG3	1:B:324:GLY:O	2.10	0.51
1:A:27:LEU:HD22	1:A:28:GLN:N	2.26	0.51
1:B:140:ILE:O	1:B:142:PRO:HD3	2.11	0.51
1:A:94:LYS:HD2	1:A:94:LYS:O	2.10	0.51
1:B:233:HIS:HE1	1:B:323:ASP:OD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:HB2	1:B:206:LYS:O	2.11	0.50
1:B:63:GLY:HA3	1:B:402:MET:HE3	1.92	0.50
1:A:155:LYS:HG3	1:A:156:GLY:N	2.25	0.50
1:B:235:LYS:HB3	1:B:237:ILE:HD13	1.91	0.50
1:A:138:TYR:CZ	1:A:457:TYR:HA	2.46	0.50
1:B:500:TYR:HB2	1:B:503:LEU:HD12	1.94	0.50
1:B:10:SER:HA	1:B:15:ALA:HB3	1.92	0.50
1:B:438:LYS:O	1:B:441:LEU:HB2	2.11	0.50
1:A:105:GLU:O	1:A:107:PRO:HD3	2.10	0.50
1:A:165:PRO:O	1:A:166:THR:HB	2.10	0.50
1:B:32:ASN:N	1:B:69:ASP:OD2	2.36	0.50
1:B:257:ASP:OD2	1:B:265:SER:HB2	2.12	0.50
1:B:195:LEU:HD23	1:B:195:LEU:N	2.27	0.50
1:A:205:HIS:O	1:A:205:HIS:ND1	2.44	0.50
1:B:496:LEU:HD21	1:B:558:LEU:HB3	1.93	0.50
1:A:444:LEU:HD11	1:A:582:LEU:HD11	1.94	0.50
1:A:385:ARG:HB3	1:A:392:MET:HE2	1.94	0.50
1:B:158:ARG:NH1	1:B:474:CYS:HB3	2.27	0.49
1:A:31:LYS:HG3	1:A:67:LEU:C	2.32	0.49
1:A:199:PHE:O	1:A:200:ARG:C	2.50	0.49
1:A:329:VAL:O	1:A:329:VAL:HG12	2.12	0.49
1:A:163:GLU:O	1:A:164:ASP:HB3	2.12	0.49
1:A:557:ASN:HD21	1:A:559:LEU:HB2	1.77	0.49
1:B:326:ARG:C	1:B:326:ARG:CD	2.80	0.49
1:A:102:PHE:C	1:A:103:TYR:CD1	2.81	0.49
1:B:158:ARG:CB	1:B:159:PRO:HD2	2.42	0.49
1:A:229:VAL:HG12	1:A:233:HIS:CD2	2.47	0.49
1:B:157:ALA:O	1:B:158:ARG:O	2.30	0.49
1:A:553:LYS:HD2	1:A:588:TRP:CG	2.46	0.49
1:A:191:THR:O	1:A:237:ILE:HA	2.13	0.49
1:A:557:ASN:HD22	1:A:558:LEU:N	2.10	0.49
1:A:400:ARG:NH1	1:A:400:ARG:HG3	2.25	0.49
1:B:511:LEU:CD1	1:B:511:LEU:N	2.76	0.49
1:A:4:GLU:CD	1:A:4:GLU:H	2.16	0.49
1:A:335:HIS:CD2	1:A:370:GLN:OE1	2.66	0.49
1:B:279:GLN:HB2	1:B:281:GLU:HG2	1.94	0.49
1:B:464:THR:OG1	1:B:465:GLY:N	2.46	0.49
1:A:1:MET:SD	1:A:90:ALA:HB3	2.52	0.49
1:A:167:PRO:CD	1:A:168:THR:H	2.26	0.49
1:B:271:PHE:CD1	1:B:271:PHE:N	2.81	0.49
1:A:288:THR:O	1:A:289:PHE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PRO:HG2	1:B:412:VAL:CG2	2.43	0.49
1:B:284:PRO:HB3	1:B:286:TYR:CD1	2.48	0.48
1:A:390:GLU:HB3	1:A:537:ARG:NH1	2.28	0.48
1:A:38:GLU:HG3	1:A:58:PRO:HB3	1.94	0.48
1:B:365:TRP:HB3	1:B:371:PHE:CD2	2.48	0.48
1:A:299:ASN:HD21	1:A:301:ALA:HB3	1.78	0.48
1:B:162:SER:C	1:B:163:GLU:HG3	2.33	0.48
1:B:209:THR:O	1:B:249:GLY:HA3	2.13	0.48
1:A:30:LYS:HB3	1:A:33:ASP:CB	2.41	0.48
1:B:137:TRP:O	1:B:455:ILE:N	2.41	0.48
1:A:48:HIS:HB3	1:A:53:GLN:NE2	2.28	0.48
1:A:243:ALA:HB3	1:A:327:LEU:HD23	1.94	0.48
1:A:131:TRP:CE3	1:A:135:THR:HG21	2.49	0.48
1:B:60:ARG:HH12	1:B:72:LEU:HD23	1.78	0.48
1:B:345:VAL:CG2	1:B:346:LYS:N	2.75	0.48
1:A:131:TRP:HE3	1:A:135:THR:HG21	1.78	0.48
1:A:302:HIS:ND1	1:A:303:PRO:HD2	2.29	0.48
1:A:1:MET:HB3	1:A:93:GLU:OE2	2.13	0.48
1:A:560:THR:HG23	1:A:562:GLU:N	2.25	0.48
1:B:546:MET:CE	1:B:571:LEU:HD23	2.44	0.48
1:A:549:ASP:OD2	1:A:551:ARG:HB2	2.13	0.48
1:B:147:ASN:HD22	1:B:147:ASN:C	2.16	0.48
1:B:41:PHE:O	1:B:54:PHE:HB2	2.14	0.48
1:B:540:GLU:C	1:B:577:PRO:HG3	2.34	0.48
1:B:160:TRP:HB3	1:B:165:PRO:CD	2.43	0.48
1:B:330:ALA:HB1	1:B:371:PHE:HZ	1.73	0.48
1:B:233:HIS:CE1	1:B:323:ASP:OD2	2.67	0.48
1:A:46:GLU:HA	1:A:46:GLU:OE1	2.13	0.48
1:B:128:ALA:O	1:B:129:PRO:O	2.32	0.48
1:B:444:LEU:CD1	1:B:582:LEU:HD11	2.44	0.48
1:B:213:PHE:HE2	1:B:308:TYR:CE1	2.32	0.48
1:A:56:THR:O	1:A:56:THR:HG23	2.14	0.48
1:B:99:GLU:HB2	1:B:115:PHE:CD1	2.49	0.48
1:B:61:LYS:HD2	1:B:69:ASP:HB3	1.95	0.47
1:B:409:PRO:HG2	1:B:412:VAL:HG23	1.96	0.47
1:B:333:ILE:HB	1:B:338:TRP:NE1	2.29	0.47
1:B:304:GLU:O	1:B:305:VAL:C	2.53	0.47
1:A:330:ALA:HB1	1:A:371:PHE:HZ	1.79	0.47
1:B:289:PHE:CZ	2:B:1589:BCD:H642	2.49	0.47
1:A:345:VAL:CG2	1:A:346:LYS:N	2.76	0.47
1:B:399:ASP:O	1:B:400:ARG:C	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:MET:O	1:A:533:ILE:HD12	2.14	0.47
1:B:237:ILE:N	1:B:237:ILE:HD12	2.29	0.47
1:B:335:HIS:CD2	1:B:370:GLN:OE1	2.67	0.47
1:A:122:ARG:O	1:A:125:LEU:HB3	2.15	0.47
1:B:401:LEU:HA	1:B:401:LEU:HD12	1.76	0.47
1:B:279:GLN:HB2	1:B:281:GLU:OE2	2.15	0.47
1:A:410:LYS:NZ	1:A:507:ASP:OD1	2.47	0.47
1:A:557:ASN:ND2	1:A:557:ASN:C	2.68	0.47
1:A:558:LEU:CD1	1:A:558:LEU:N	2.78	0.47
1:A:131:TRP:CZ3	1:A:238:ARG:HG3	2.49	0.47
1:B:271:PHE:HB2	1:B:273:ILE:HD11	1.96	0.47
1:A:188:LEU:HD23	1:A:188:LEU:O	2.14	0.47
1:B:276:PHE:C	1:B:278:LEU:H	2.17	0.47
1:A:426:PRO:HA	1:A:466:GLY:O	2.15	0.47
1:B:409:PRO:O	1:B:412:VAL:HB	2.14	0.47
1:A:233:HIS:HE1	1:A:323:ASP:OD2	1.97	0.47
1:A:517:VAL:O	1:A:517:VAL:HG12	2.13	0.47
1:B:209:THR:O	1:B:249:GLY:N	2.48	0.47
1:A:197:PRO:HB2	1:A:206:LYS:HB3	1.97	0.47
1:A:427:ARG:NH1	1:A:456:TYR:CD2	2.83	0.47
1:B:1:MET:SD	1:B:34:VAL:HG22	2.54	0.47
1:B:560:THR:HG22	1:B:562:GLU:HB2	1.96	0.47
1:A:23:LEU:HD21	1:A:117:PHE:CE1	2.49	0.47
1:A:281:GLU:CB	1:A:282:PRO:CD	2.83	0.46
1:B:540:GLU:CA	1:B:577:PRO:HG3	2.46	0.46
1:A:558:LEU:HD12	1:A:558:LEU:N	2.30	0.46
1:B:206:LYS:HE2	1:B:219:PHE:CE2	2.51	0.46
1:B:78:PRO:O	1:B:79:TYR:HB2	2.15	0.46
1:B:167:PRO:CG	1:B:168:THR:H	2.28	0.46
1:B:12:ASP:OD2	1:B:367:ARG:NH1	2.49	0.46
1:B:150:PRO:C	1:B:152:ILE:H	2.17	0.46
1:A:1:MET:CE	1:A:95:LEU:HD22	2.44	0.46
1:A:523:ALA:HB2	1:A:532:MET:SD	2.55	0.46
1:B:34:VAL:HG13	1:B:89:ARG:O	2.15	0.46
1:B:272:HIS:HB2	1:B:287:ASP:HB2	1.97	0.46
1:A:528:ASN:N	1:A:528:ASN:ND2	2.63	0.46
1:B:166:THR:HG22	1:B:469:PRO:HB2	1.97	0.46
1:A:290:ALA:O	1:A:291:PHE:CG	2.69	0.46
1:B:48:HIS:O	1:B:49:ASP:HB2	2.16	0.46
1:A:501:ARG:HD3	1:A:526:ASP:OD2	2.16	0.46
1:A:400:ARG:O	1:A:404:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:O	1:B:345:VAL:HG22	2.16	0.46
1:A:423:HIS:HB2	1:A:472:ARG:HE	1.80	0.46
1:B:379:LEU:HD23	1:B:379:LEU:C	2.36	0.46
1:A:419:LEU:HD23	1:A:419:LEU:N	2.23	0.46
1:B:558:LEU:HD22	1:B:582:LEU:HB3	1.98	0.45
1:A:27:LEU:CD2	1:A:28:GLN:N	2.79	0.45
1:B:369:ASP:C	1:B:370:GLN:HG3	2.36	0.45
1:A:5:ALA:HB2	1:B:4:GLU:HB3	1.97	0.45
1:A:355:LEU:HD12	1:A:356:GLY:N	2.31	0.45
1:B:155:LYS:HE2	1:B:172:GLY:N	2.31	0.45
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.81	0.45
1:B:439:VAL:HG11	1:B:486:LEU:HD21	1.98	0.45
1:A:158:ARG:HB3	1:A:159:PRO:CD	2.38	0.45
1:B:188:LEU:HD11	1:B:460:GLU:HG2	1.96	0.45
1:B:248:CYS:SG	1:B:296:PRO:HG2	2.56	0.45
1:B:195:LEU:HD23	1:B:195:LEU:H	1.82	0.45
1:A:588:TRP:C	1:A:588:TRP:CD2	2.89	0.45
1:B:341:PHE:HE2	1:B:354:ILE:HG23	1.81	0.45
1:A:448:THR:CG2	1:A:522:TYR:OH	2.64	0.45
1:B:54:PHE:CD1	1:B:54:PHE:C	2.89	0.45
1:B:486:LEU:O	1:B:489:HIS:HB3	2.15	0.45
1:A:44:PRO:HG3	1:A:83:ARG:HG2	1.98	0.45
1:A:208:ASP:N	1:A:208:ASP:OD2	2.48	0.45
1:B:256:GLN:O	1:B:259:LEU:HB2	2.17	0.45
1:A:82:LEU:O	1:A:82:LEU:HD23	2.16	0.45
1:A:404:VAL:HG23	1:A:405:LEU:H	1.82	0.45
1:B:376:ASN:C	1:B:378:PRO:HD2	2.36	0.45
1:B:30:LYS:HB3	1:B:33:ASP:CB	2.47	0.45
1:A:261:ASN:HB3	1:A:264:ALA:HB3	1.97	0.45
1:A:159:PRO:HD3	1:A:474:CYS:HB2	1.99	0.45
1:A:140:ILE:O	1:A:142:PRO:N	2.49	0.45
1:B:159:PRO:HA	1:B:165:PRO:HG2	1.98	0.45
1:B:37:VAL:HG13	1:B:37:VAL:O	2.16	0.45
1:B:215:ILE:O	1:B:216:ASP:C	2.54	0.45
1:A:35:ASP:OD2	1:A:91:GLY:N	2.45	0.45
1:A:132:VAL:HA	1:A:135:THR:HG23	1.99	0.45
1:A:349:LYS:HB3	1:A:352:VAL:CG2	2.47	0.45
1:A:201:ALA:HB1	1:A:202:PRO:HD2	1.99	0.45
1:A:37:VAL:HG23	1:A:88:LEU:HB3	2.00	0.45
1:A:168:THR:HG22	1:A:168:THR:O	2.17	0.45
1:B:552:GLY:HA2	1:B:587:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PRO:CG	1:B:168:THR:N	2.79	0.45
1:B:142:PRO:O	1:B:173:GLY:HA3	2.17	0.45
1:B:243:ALA:HB3	1:B:327:LEU:HD23	1.98	0.44
1:B:327:LEU:HD13	1:B:338:TRP:CZ3	2.52	0.44
1:A:82:LEU:C	1:A:82:LEU:HD23	2.37	0.44
1:A:1:MET:CE	1:A:95:LEU:HB2	2.47	0.44
1:A:16:TYR:CD2	1:A:409:PRO:HB3	2.51	0.44
1:B:483:ASN:OD1	1:B:485:GLU:HB3	2.17	0.44
1:B:431:VAL:HG12	1:B:431:VAL:O	2.18	0.44
1:A:306:LYS:O	1:A:310:LEU:HB2	2.17	0.44
1:B:153:SER:H	1:B:155:LYS:HZ2	1.64	0.44
1:B:557:ASN:CG	1:B:560:THR:HB	2.37	0.44
1:B:175:LEU:O	1:B:176:GLN:C	2.53	0.44
1:B:80:ARG:CG	1:B:80:ARG:HH11	2.29	0.44
1:B:1:MET:SD	1:B:90:ALA:HB2	2.56	0.44
1:A:6:ILE:HA	1:A:28:GLN:O	2.18	0.44
1:B:167:PRO:HG2	1:B:168:THR:N	2.33	0.44
1:B:555:LEU:CD1	1:B:585:VAL:HG22	2.48	0.44
1:B:164:ASP:HB2	1:B:165:PRO:CD	2.41	0.44
1:A:444:LEU:O	1:A:448:THR:HG22	2.18	0.44
1:A:328:ASP:OD2	1:A:329:VAL:HG23	2.17	0.44
1:B:279:GLN:HB2	1:B:281:GLU:CG	2.48	0.44
1:A:199:PHE:CE1	1:A:316:TRP:CZ2	3.06	0.44
1:A:345:VAL:HG23	1:A:346:LYS:H	1.82	0.44
1:A:585:VAL:HG12	1:A:586:GLU:N	2.32	0.44
1:A:290:ALA:O	1:B:81:ARG:NH2	2.49	0.44
1:B:160:TRP:HB3	1:B:165:PRO:HG3	1.99	0.44
1:A:276:PHE:O	1:A:278:LEU:N	2.50	0.44
1:A:531:VAL:HG12	1:A:533:ILE:CD1	2.48	0.44
1:B:165:PRO:O	1:B:166:THR:CB	2.65	0.43
1:A:304:GLU:O	1:A:305:VAL:C	2.57	0.43
1:A:179:ILE:O	1:A:182:LEU:HB2	2.18	0.43
1:B:37:VAL:HG11	1:B:71:TRP:CG	2.53	0.43
1:A:161:GLY:H	1:A:165:PRO:HG3	1.83	0.43
1:A:534:ILE:HG21	1:A:573:VAL:HG11	1.98	0.43
1:B:30:LYS:HB3	1:B:33:ASP:HB2	1.98	0.43
1:B:564:PHE:CD1	1:B:564:PHE:N	2.86	0.43
1:B:155:LYS:HE2	1:B:171:PHE:C	2.39	0.43
1:A:253:ALA:CB	1:A:254:PRO:CD	2.92	0.43
1:A:559:LEU:HD11	1:A:580:PHE:CE1	2.51	0.43
1:A:448:THR:O	1:A:448:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD12	1:A:84:TYR:CE2	2.53	0.43
1:B:38:GLU:OE2	1:B:89:ARG:NE	2.42	0.43
1:B:427:ARG:NH1	1:B:457:TYR:O	2.47	0.43
1:B:362:ALA:HB3	1:B:374:VAL:HG21	2.01	0.43
1:A:181:HIS:O	1:A:184:TYR:HB3	2.18	0.43
1:B:365:TRP:HB3	1:B:371:PHE:HD2	1.82	0.43
1:B:327:LEU:HD13	1:B:371:PHE:HE1	1.83	0.43
1:B:377:TYR:N	1:B:378:PRO:CD	2.82	0.43
1:B:37:VAL:HG13	1:B:59:MET:HE3	2.01	0.43
1:A:327:LEU:HD11	1:A:354:ILE:CG2	2.48	0.43
1:B:385:ARG:HH11	1:B:392:MET:CE	2.29	0.43
1:B:531:VAL:HG12	1:B:533:ILE:HD11	2.01	0.43
1:A:457:TYR:O	1:A:460:GLU:OE2	2.36	0.43
1:A:335:HIS:O	1:A:339:ARG:HG3	2.18	0.43
1:B:574:SER:C	1:B:575:LEU:HD12	2.38	0.43
1:A:435:ASP:OD1	1:A:437:ARG:HB2	2.17	0.43
1:A:59:MET:HE1	1:A:86:PHE:CD2	2.42	0.43
1:A:476:VAL:O	1:A:482:GLN:NE2	2.51	0.43
1:B:194:TYR:C	1:B:194:TYR:CD1	2.92	0.43
1:A:161:GLY:H	1:A:165:PRO:CG	2.31	0.43
1:B:333:ILE:HB	1:B:338:TRP:HE1	1.84	0.43
1:A:463:MET:SD	1:A:476:VAL:HG23	2.59	0.43
1:B:521:VAL:HG13	1:B:521:VAL:O	2.19	0.43
1:B:534:ILE:HD11	1:B:546:MET:SD	2.58	0.43
1:B:200:ARG:HA	1:B:216:ASP:HA	2.01	0.43
1:A:194:TYR:C	1:A:194:TYR:CD1	2.92	0.43
1:A:245:PHE:CD1	1:A:309:LEU:HD22	2.54	0.43
1:B:277:PRO:O	1:B:278:LEU:C	2.57	0.43
1:A:511:LEU:HD23	1:A:547:PRO:HG2	2.01	0.43
1:A:43:ASP:OD2	1:A:81:ARG:HD3	2.19	0.43
1:B:148:GLY:O	1:B:149:ASN:C	2.56	0.43
1:A:564:PHE:N	1:A:564:PHE:CD1	2.86	0.43
1:B:88:LEU:N	1:B:88:LEU:CD2	2.79	0.42
1:B:557:ASN:HD21	1:B:559:LEU:H	1.63	0.42
1:A:206:LYS:HE2	1:A:219:PHE:CZ	2.54	0.42
1:A:273:ILE:HD12	1:A:273:ILE:H	1.82	0.42
1:A:237:ILE:N	1:A:237:ILE:CD1	2.82	0.42
1:B:456:TYR:O	1:B:457:TYR:C	2.57	0.42
1:A:2:ARG:HH22	1:B:2:ARG:HD2	1.83	0.42
1:A:150:PRO:C	1:A:152:ILE:H	2.22	0.42
1:B:250:TYR:HB2	1:B:294:HIS:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:CD1	1:B:178:ILE:HG12	2.50	0.42
1:A:309:LEU:O	1:A:312:VAL:N	2.53	0.42
1:A:30:LYS:HG2	1:A:31:LYS:N	2.35	0.42
1:B:477:TRP:O	1:B:479:PRO:HD3	2.19	0.42
1:B:326:ARG:HH12	1:B:375:MET:HE2	1.84	0.42
1:B:460:GLU:CD	1:B:460:GLU:H	2.22	0.42
1:B:205:HIS:C	1:B:205:HIS:ND1	2.73	0.42
1:B:2:ARG:HH11	1:B:2:ARG:HG3	1.83	0.42
1:B:363:MET:CB	1:B:364:PRO:HD3	2.50	0.42
1:B:43:ASP:HB3	1:B:46:GLU:HB2	2.02	0.42
1:B:450:THR:CG2	1:B:505:ARG:HA	2.46	0.42
1:B:207:TYR:C	1:B:209:THR:H	2.22	0.42
1:A:502:ALA:HB2	1:A:529:GLU:HG2	2.01	0.42
1:A:478:ASP:O	1:A:481:LYS:N	2.46	0.42
1:B:253:ALA:CB	1:B:254:PRO:HD3	2.35	0.42
1:A:466:GLY:N	1:A:470:GLU:HB3	2.35	0.42
1:A:80:ARG:HD2	1:A:119:PHE:CZ	2.55	0.42
1:B:177:GLY:O	1:B:178:ILE:C	2.58	0.42
1:A:1:MET:HE1	1:A:95:LEU:HB2	2.01	0.42
1:A:534:ILE:CD1	1:A:573:VAL:HG11	2.48	0.42
1:B:224:THR:O	1:B:227:THR:HB	2.19	0.42
1:B:27:LEU:HD22	1:B:28:GLN:N	2.35	0.42
1:A:273:ILE:HG23	1:A:286:TYR:HB3	2.01	0.42
1:A:528:ASN:N	1:A:528:ASN:HD22	2.17	0.42
1:A:326:ARG:C	1:A:326:ARG:HD2	2.40	0.42
1:B:435:ASP:OD1	1:B:437:ARG:HB2	2.19	0.42
1:A:345:VAL:HG21	1:A:354:ILE:HD11	2.02	0.42
1:A:573:VAL:CG1	1:A:573:VAL:O	2.68	0.42
1:A:304:GLU:O	1:A:307:ARG:N	2.53	0.42
1:A:161:GLY:N	1:A:165:PRO:HG3	2.35	0.42
1:A:293:PRO:C	1:A:295:MET:H	2.24	0.42
1:A:62:THR:OG1	1:A:406:HIS:HE1	2.02	0.42
1:B:163:GLU:HB3	1:B:473:LYS:HZ1	1.85	0.42
1:B:302:HIS:CD2	1:B:304:GLU:HB2	2.54	0.42
1:B:288:THR:HG22	1:B:296:PRO:HA	2.02	0.42
1:B:299:ASN:C	1:B:301:ALA:H	2.23	0.42
1:B:245:PHE:CD1	1:B:245:PHE:N	2.88	0.42
1:B:528:ASN:HA	1:B:528:ASN:HD22	1.56	0.42
1:A:513:ALA:C	1:A:515:ASP:N	2.74	0.41
1:B:147:ASN:ND2	1:B:148:GLY:O	2.53	0.41
1:B:541:ALA:N	1:B:577:PRO:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TYR:CZ	1:B:457:TYR:HA	2.55	0.41
1:B:575:LEU:HD21	1:B:581:VAL:HG12	2.02	0.41
1:B:10:SER:HB3	1:B:84:TYR:OH	2.20	0.41
1:A:182:LEU:HG	1:A:235:LYS:NZ	2.35	0.41
1:B:349:LYS:HB3	1:B:352:VAL:HG23	2.02	0.41
1:A:418:ASN:O	1:A:453:PRO:HA	2.20	0.41
1:B:167:PRO:HG2	1:B:168:THR:H	1.85	0.41
2:A:1589:BCD:HO61	1:B:45:TYR:HD2	1.64	0.41
1:A:289:PHE:CE1	2:A:1589:BCD:H642	2.56	0.41
1:B:225:LEU:O	1:B:226:LYS:C	2.58	0.41
1:A:328:ASP:CG	1:A:329:VAL:HG23	2.40	0.41
1:B:577:PRO:O	1:B:578:TYR:HB2	2.21	0.41
1:B:138:TYR:OH	1:B:457:TYR:HA	2.21	0.41
1:B:276:PHE:C	1:B:278:LEU:N	2.74	0.41
1:A:345:VAL:CG2	1:A:346:LYS:H	2.33	0.41
1:A:548:ILE:HG21	1:A:566:ALA:HB1	2.01	0.41
1:A:466:GLY:H	1:A:470:GLU:HB3	1.85	0.41
1:A:281:GLU:O	1:A:282:PRO:C	2.56	0.41
1:A:558:LEU:HD11	1:A:584:ALA:CB	2.49	0.41
1:B:63:GLY:HA3	1:B:402:MET:HE2	1.99	0.41
1:A:430:THR:HG21	1:A:465:GLY:O	2.21	0.41
1:B:295:MET:SD	2:B:1589:BCD:H652	2.60	0.41
1:A:404:VAL:HG23	1:A:405:LEU:N	2.35	0.41
1:A:197:PRO:HB2	1:A:206:LYS:CB	2.50	0.41
1:B:24:HIS:C	1:B:25:LEU:HD22	2.41	0.41
1:B:59:MET:HG2	1:B:73:ALA:HB2	2.02	0.41
1:B:333:ILE:HG22	1:B:334:ASP:N	2.36	0.41
1:A:573:VAL:HG13	1:A:573:VAL:O	2.21	0.41
1:A:430:THR:HG23	1:A:465:GLY:H	1.81	0.41
1:B:305:VAL:O	1:B:308:TYR:HB3	2.21	0.41
1:B:47:TRP:O	1:B:48:HIS:HB2	2.21	0.41
1:A:437:ARG:O	1:A:440:LYS:HG3	2.21	0.41
1:B:122:ARG:O	1:B:125:LEU:HB3	2.21	0.41
1:B:153:SER:N	1:B:155:LYS:HZ2	2.19	0.41
1:A:158:ARG:CB	1:A:159:PRO:CD	2.95	0.41
1:B:385:ARG:NH1	1:B:392:MET:HE3	2.32	0.41
1:B:207:TYR:HD1	1:B:244:VAL:CG2	2.34	0.41
1:A:137:TRP:O	1:A:454:CYS:HA	2.21	0.41
1:B:557:ASN:ND2	1:B:559:LEU:HD12	2.19	0.40
1:A:160:TRP:HB3	1:A:165:PRO:CG	2.51	0.40
1:A:461:ILE:CD1	1:A:463:MET:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:OE1	1:A:423:HIS:HD2	2.03	0.40
1:A:501:ARG:N	1:A:529:GLU:OE2	2.54	0.40
1:A:9:ARG:HD3	1:B:361:ASP:OD2	2.21	0.40
1:B:448:THR:HG22	1:B:448:THR:O	2.21	0.40
1:B:519:HIS:ND1	1:B:544:ILE:HG12	2.35	0.40
1:B:158:ARG:HA	1:B:158:ARG:HD3	1.89	0.40
1:A:533:ILE:HD12	1:A:533:ILE:N	2.35	0.40
1:A:84:TYR:N	1:A:84:TYR:CD1	2.89	0.40
1:B:401:LEU:HD23	1:B:510:PHE:CZ	2.56	0.40
1:B:125:LEU:HD12	1:B:126:PHE:N	2.36	0.40
1:A:420:LEU:HG	1:A:446:GLN:OE1	2.21	0.40
1:B:276:PHE:O	1:B:278:LEU:N	2.44	0.40
1:A:585:VAL:O	1:A:586:GLU:OE1	2.39	0.40
1:A:521:VAL:HG13	1:A:521:VAL:O	2.20	0.40
1:B:162:SER:O	1:B:163:GLU:HG3	2.21	0.40
1:A:477:TRP:O	1:A:479:PRO:HD3	2.21	0.40
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.90	0.40
1:A:231:ARG:O	1:A:234:GLU:HB3	2.21	0.40
1:B:199:PHE:CE1	1:B:316:TRP:CZ2	3.08	0.40
1:B:128:ALA:O	1:B:129:PRO:C	2.60	0.40
1:A:65:ASP:HB2	1:A:66:GLY:H	1.70	0.40
1:A:61:LYS:HD2	1:A:69:ASP:OD2	2.22	0.40
1:A:588:TRP:OXT	1:A:588:TRP:CG	2.75	0.40
1:A:419:LEU:CD2	1:A:419:LEU:H	2.27	0.40
1:B:57:MET:HE1	1:B:75:VAL:HG23	2.02	0.40
1:A:302:HIS:CD2	1:A:304:GLU:H	2.40	0.40
1:B:401:LEU:HD21	1:B:445:PHE:CZ	2.57	0.40
1:B:435:ASP:O	1:B:437:ARG:N	2.54	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	586/588 (100%)	486 (83%)	76 (13%)	24 (4%)	3 24
1	B	586/588 (100%)	467 (80%)	93 (16%)	26 (4%)	3 22
All	All	1172/1176 (100%)	953 (81%)	169 (14%)	50 (4%)	3 23

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	118	PRO
1	A	156	GLY
1	A	158	ARG
1	A	159	PRO
1	A	164	ASP
1	A	166	THR
1	A	167	PRO
1	A	168	THR
1	A	281	GLU
1	A	289	PHE
1	A	457	TYR
1	B	158	ARG
1	B	159	PRO
1	B	167	PRO
1	B	168	THR
1	B	170	PHE
1	B	265	SER
1	B	281	GLU
1	B	289	PHE
1	B	360	HIS
1	A	265	SER
1	B	118	PRO
1	B	160	TRP
1	B	209	THR
1	B	483	ASN
1	A	12	ASP
1	A	13	ASN
1	A	20	SER
1	A	174	ASP
1	A	278	LEU
1	A	291	PHE
1	B	129	PRO
1	B	165	PRO
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	278	LEU
1	A	200	ARG
1	B	11	THR
1	B	48	HIS
1	B	166	THR
1	B	566	ALA
1	A	141	PHE
1	A	155	LYS
1	A	514	ASP
1	A	567	GLU
1	B	274	ARG
1	B	436	VAL
1	B	551	ARG
1	B	316	TRP
1	B	142	PRO

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	505/505 (100%)	452 (90%)	53 (10%)	8 33
1	B	505/505 (100%)	457 (90%)	48 (10%)	11 38
All	All	1010/1010 (100%)	909 (90%)	101 (10%)	9 36

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	26	ARG
1	A	27	LEU
1	A	47	TRP
1	A	49	ASP
1	A	69	ASP
1	A	81	ARG
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	94	LYS
1	A	135	THR
1	A	147	ASN
1	A	159	PRO
1	A	163	GLU
1	A	170	PHE
1	A	183	ASP
1	A	188	LEU
1	A	194	TYR
1	A	196	THR
1	A	200	ARG
1	A	209	THR
1	A	230	LYS
1	A	235	LYS
1	A	260	LYS
1	A	266	ARG
1	A	268	LYS
1	A	273	ILE
1	A	276	PHE
1	A	280	THR
1	A	281	GLU
1	A	298	LEU
1	A	299	ASN
1	A	307	ARG
1	A	310	LEU
1	A	311	ASP
1	A	314	THR
1	A	326	ARG
1	A	348	LEU
1	A	359	TRP
1	A	363	MET
1	A	389	LYS
1	A	440	LYS
1	A	446	GLN
1	A	460	GLU
1	A	471	CYS
1	A	520	LEU
1	A	525	THR
1	A	556	VAL
1	A	557	ASN
1	A	560	THR

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Mol	Chain	Res	Type
1	A	573	VAL
1	A	586	GLU
1	A	588	TRP
1	B	9	ARG
1	B	24	HIS
1	B	27	LEU
1	B	47	TRP
1	B	60	ARG
1	B	61	LYS
1	B	67	LEU
1	B	80	ARG
1	B	81	ARG
1	B	88	LEU
1	B	110	ASP
1	B	123	VAL
1	B	147	ASN
1	B	155	LYS
1	B	159	PRO
1	B	194	TYR
1	B	195	LEU
1	B	196	THR
1	B	200	ARG
1	B	235	LYS
1	B	268	LYS
1	B	276	PHE
1	B	299	ASN
1	B	300	THR
1	B	310	LEU
1	B	314	THR
1	B	326	ARG
1	B	348	LEU
1	B	359	TRP
1	B	363	MET
1	B	374	VAL
1	B	379	LEU
1	B	385	ARG
1	B	401	LEU
1	B	404	VAL
1	B	407	SER
1	B	428	LEU
1	B	460	GLU
1	B	464	THR

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Mol	Chain	Res	Type
1	B	499	GLN
1	B	525	THR
1	B	528	ASN
1	B	537	ARG
1	B	557	ASN
1	B	559	LEU
1	B	563	ARG
1	B	570	THR
1	B	588	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	32	ASN
1	A	53	GLN
1	A	139	GLN
1	A	147	ASN
1	A	149	ASN
1	A	181	HIS
1	A	233	HIS
1	A	272	HIS
1	A	279	GLN
1	A	299	ASN
1	A	302	HIS
1	A	335	HIS
1	A	360	HIS
1	A	406	HIS
1	A	418	ASN
1	A	423	HIS
1	A	482	GLN
1	A	499	GLN
1	A	518	ASN
1	A	528	ASN
1	A	557	ASN
1	B	7	HIS
1	B	24	HIS
1	B	32	ASN
1	B	139	GLN
1	B	147	ASN
1	B	233	HIS
1	B	299	ASN

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Mol	Chain	Res	Type
1	B	302	HIS
1	B	335	HIS
1	B	343	GLN
1	B	360	HIS
1	B	370	GLN
1	B	406	HIS
1	B	418	ASN
1	B	423	HIS
1	B	482	GLN
1	B	499	GLN
1	B	528	ASN
1	B	557	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

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	BCD	A	1589	-	84,84,84	1.88	6 (7%)	126,126,126	1.71	15 (11%)
2	BCD	B	1589	-	84,84,84	1.90	6 (7%)	126,126,126	1.69	15 (11%)

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	BCD	A	1589	-	-	0/42/182/182	0/0/8/8
2	BCD	B	1589	-	-	0/42/182/182	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1589	BCD	O47-C11	-12.98	1.06	1.41
2	A	1589	BCD	O47-C11	-12.94	1.06	1.41
2	B	1589	BCD	O44-C15	-4.13	1.30	1.41
2	A	1589	BCD	O44-C15	-4.01	1.30	1.41
2	B	1589	BCD	O52-C12	2.02	1.47	1.41
2	A	1589	BCD	O57-C17	2.02	1.47	1.41
2	A	1589	BCD	O52-C12	2.05	1.47	1.41
2	A	1589	BCD	O46-C17	2.21	1.47	1.41
2	B	1589	BCD	O47-C47	2.47	1.50	1.43
2	B	1589	BCD	O46-C17	2.62	1.48	1.41
2	B	1589	BCD	O42-C13	4.13	1.52	1.41
2	A	1589	BCD	O42-C13	4.38	1.53	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1589	BCD	O41-C12-C22	-6.56	92.15	108.10
2	B	1589	BCD	O41-C12-C22	-5.90	93.74	108.10
2	A	1589	BCD	O44-C15-O55	-5.46	96.85	110.68
2	B	1589	BCD	O44-C15-O55	-5.22	97.48	110.68
2	B	1589	BCD	C14-O43-C43	-4.64	105.87	118.01
2	A	1589	BCD	C14-O43-C43	-4.20	107.02	118.01
2	B	1589	BCD	O43-C43-C53	-3.92	99.02	109.32
2	A	1589	BCD	O43-C43-C53	-3.78	99.39	109.32
2	B	1589	BCD	O42-C42-C32	-3.67	97.69	107.17
2	A	1589	BCD	O42-C42-C32	-3.60	97.86	107.17
2	A	1589	BCD	O47-C11-O51	-3.54	101.72	110.68
2	B	1589	BCD	O47-C11-O51	-3.17	102.65	110.68
2	A	1589	BCD	C12-O41-C41	-2.65	111.08	118.01
2	B	1589	BCD	C12-O41-C41	-2.52	111.43	118.01
2	A	1589	BCD	O63-C63-C53	-2.28	103.80	111.33
2	B	1589	BCD	O63-C63-C53	-2.11	104.35	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1589	BCD	C15-O44-C44	3.00	125.85	118.01
2	B	1589	BCD	O42-C42-C52	3.03	117.29	109.32
2	A	1589	BCD	O42-C42-C52	3.13	117.55	109.32
2	B	1589	BCD	C15-O44-C44	3.16	126.27	118.01
2	A	1589	BCD	C13-O42-C42	3.87	128.12	118.01
2	B	1589	BCD	C13-O42-C42	3.89	128.16	118.01
2	A	1589	BCD	O47-C11-C21	4.24	118.42	108.10
2	B	1589	BCD	O47-C11-C21	4.46	118.94	108.10
2	B	1589	BCD	O44-C15-C25	4.65	119.42	108.10
2	A	1589	BCD	O44-C15-C25	4.87	119.95	108.10
2	B	1589	BCD	O41-C12-O52	4.94	123.20	110.68
2	A	1589	BCD	O41-C12-O52	5.20	123.85	110.68
2	A	1589	BCD	O42-C13-C23	8.34	128.41	108.10
2	B	1589	BCD	O42-C13-C23	8.59	129.01	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1589	BCD	2	0
2	B	1589	BCD	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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