Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 10:20 AM EDT

PDB ID	:	1PV6
Title	:	Crystal structure of lactose permease
Authors	:	Abramson, J.; Smirnova, I.; Kasho, V.; Verner, G.; Kaback, H.R.; Iwata, S.
Deposited on	:	2003-06-26
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

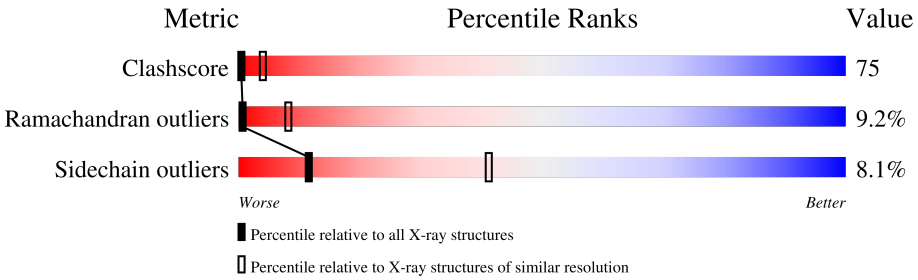
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	417	22% 64% 13%
1	B	417	23% 63% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6580 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 Lactose permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			
1	B	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	engineered mutation	UNP P02920
B	154	GLY	CYS	engineered mutation	UNP P02920

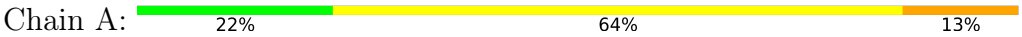
3 Residue-property plots (i)

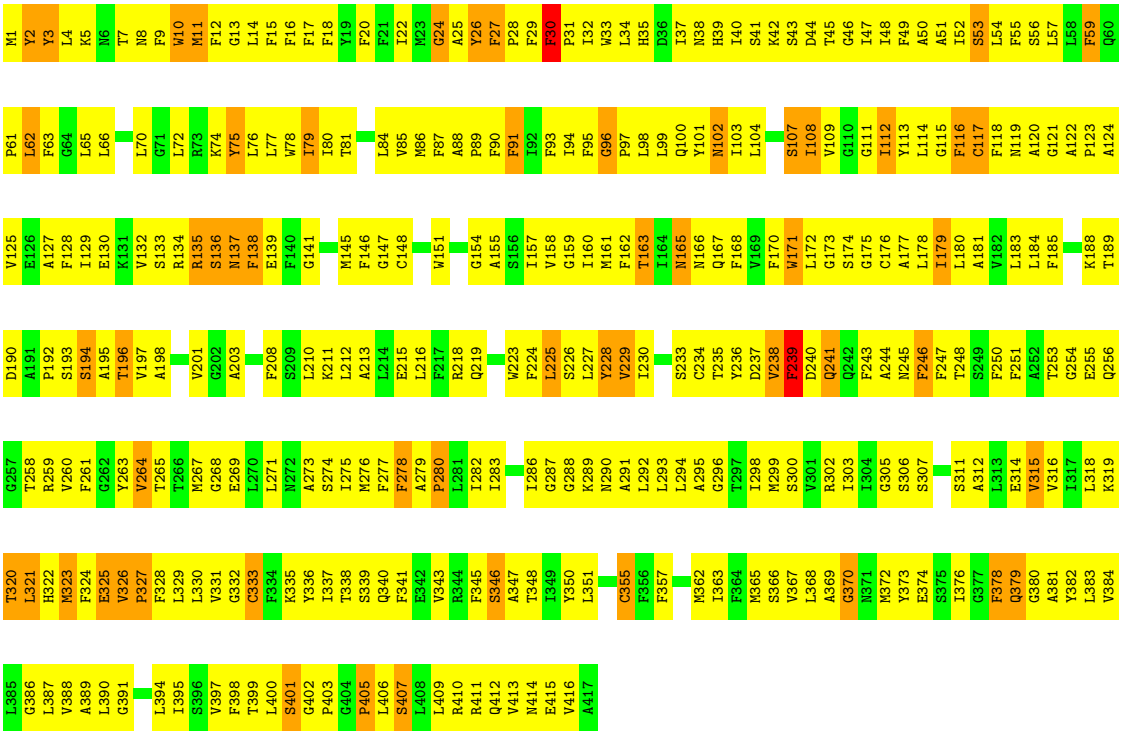
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Lactose permease

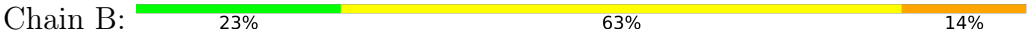
Chain A:

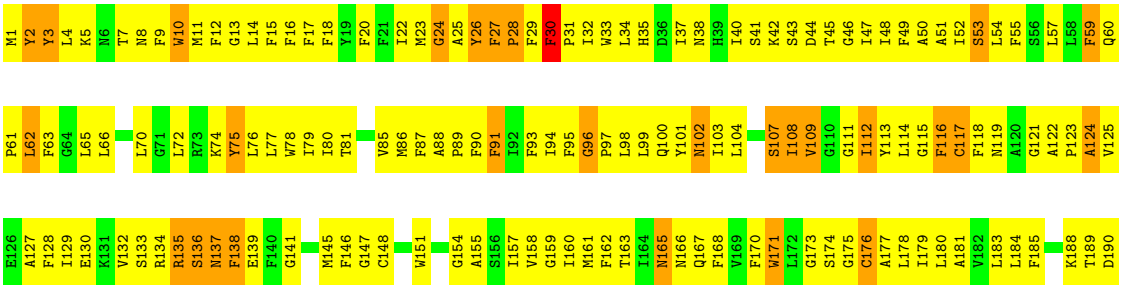


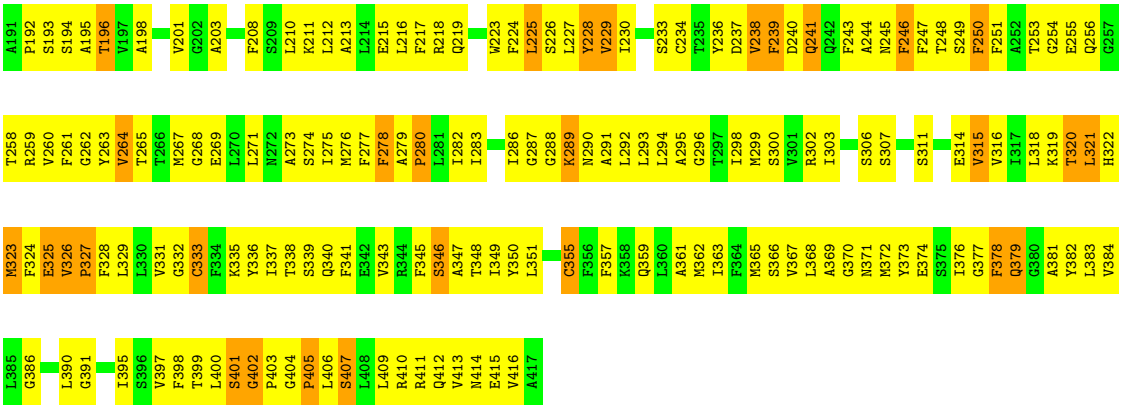


• Molecule 1: Lactose permease

Chain B:






A191 P192 S193 S194 A195 T196 V197 A198 V201 G202 A203 F208 S209 L210 K211 L212 A213 L214 E215 L216 F217 R218 Q219 W223 F224 L225 S226 L227 Y228 V229 I230 S233 C234 T235 Y236 D237 V238 F239 D240 Q241 Q242 F243 A244 N245 F246 F247 T248 S249 F250 F251 A252 T253 G254 E255 Q256 G257
T258 R259 V260 F261 G262 Y263 V264 T265 T266 M267 G268 E269 L270 L271 N272 A273 S274 I275 M276 F277 F278 A279 P280 L281 I282 I283 I286 G287 G288 K289 N290 A291 L292 L293 L294 A295 G296 T297 I298 M299 S300 V301 R302 I303 S306 S307 S311 E314 V315 V316 I317 L318 K319 T320 L321 H322
M323 F324 E325 V326 P327 F328 L329 L330 V331 G332 C333 F334 K335 Y336 I337 T338 S339 Q340 F341 E342 V343 R344 F345 S346 A347 T348 I349 Y350 L351 C355 F356 F357 K358 Q359 L360 A361 M362 I363 F364 M365 S366 V367 L368 A369 G370 N371 M372 Y373 E374 S375 I376 G377 F378 Q379 G380 A381 Y382 L383 V384
L385 G386 L390 G391 I395 S396 V397 F398 T399 L400 S401 G402 P403 G404 P405 L406 S407 L408 L409 R410 R411 Q412 V413 N414 E415 V416 A417

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.35Å 125.84Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.294 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	0/3387	0.83	2/4588 (0.0%)
1	B	0.69	1/3387 (0.0%)	0.82	2/4588 (0.0%)
All	All	0.69	1/6774 (0.0%)	0.82	4/9176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	CYS	CB-SG	-6.03	1.72	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	ASP	N-CA-C	5.61	126.15	111.00
1	A	225	LEU	CA-CB-CG	-5.48	102.70	115.30
1	B	190	ASP	N-CA-C	5.22	125.08	111.00
1	B	225	LEU	CA-CB-CG	-5.12	103.52	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	3290	0	3333	514	0
1	B	3290	0	3333	494	0
All	All	6580	0	6666	999	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 75.

All (999) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:HG3	1:B:400:LEU:HD23	1.33	1.08
1:B:30:PHE:HB3	1:B:31:PRO:HD3	1.36	1.07
1:A:289:LYS:HG3	1:A:400:LEU:HD23	1.32	1.06
1:A:30:PHE:HB3	1:A:31:PRO:HD3	1.36	1.03
1:B:180:LEU:O	1:B:184:LEU:HG	1.65	0.97
1:A:264:VAL:HG11	1:A:319:LYS:HG2	1.46	0.96
1:B:52:ILE:HA	1:B:112:ILE:HG21	1.47	0.96
1:B:33:TRP:HA	1:B:37:ILE:HD12	1.45	0.94
1:A:34:LEU:HD13	1:A:40:ILE:HD13	1.49	0.94
1:A:180:LEU:O	1:A:184:LEU:HG	1.68	0.94
1:A:196:THR:HG21	1:A:201:VAL:HB	1.49	0.93
1:A:52:ILE:HA	1:A:112:ILE:HG21	1.48	0.93
1:B:196:THR:HG21	1:B:201:VAL:HB	1.50	0.93
1:B:77:LEU:HD12	1:B:80:ILE:HD12	1.48	0.93
1:A:20:PHE:HD2	1:A:151:TRP:HB2	1.32	0.93
1:A:77:LEU:HD12	1:A:80:ILE:HD12	1.50	0.92
1:B:264:VAL:HG11	1:B:319:LYS:HG2	1.51	0.92
1:B:20:PHE:HD2	1:B:151:TRP:HB2	1.35	0.92
1:B:246:PHE:HB2	1:B:378:PHE:CD2	2.05	0.91
1:B:81:THR:O	1:B:85:VAL:HG23	1.71	0.91
1:A:90:PHE:CD1	1:A:94:ILE:HD12	2.06	0.90
1:B:409:LEU:O	1:B:413:VAL:HG23	1.72	0.90
1:A:326:VAL:HB	1:A:327:PRO:CD	2.02	0.89
1:A:37:ILE:HD13	1:A:166:ASN:HD22	1.36	0.89
1:A:50:ALA:HB2	1:A:366:SER:HB2	1.54	0.89
1:B:50:ALA:HB2	1:B:366:SER:HB2	1.55	0.89
1:B:90:PHE:CD1	1:B:94:ILE:HD12	2.08	0.88
1:B:234:CYS:SG	1:B:365:MET:SD	2.71	0.88
1:A:33:TRP:HA	1:A:37:ILE:HD12	1.54	0.87
1:A:90:PHE:CG	1:A:114:LEU:HD13	2.10	0.86
1:B:326:VAL:HB	1:B:327:PRO:CD	2.05	0.86
1:A:409:LEU:O	1:A:413:VAL:HG23	1.76	0.86
1:B:256:GLN:OE1	1:B:259:ARG:HD2	1.76	0.85
1:A:256:GLN:OE1	1:A:259:ARG:HD2	1.75	0.85
1:B:34:LEU:HD13	1:B:40:ILE:HD13	1.58	0.85
1:A:246:PHE:HB2	1:A:378:PHE:CD2	2.10	0.85
1:B:27:PHE:HB3	1:B:28:PRO:CD	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB2	1:B:3:TYR:CE1	2.12	0.84
1:B:279:ALA:HB3	1:B:280:PRO:HD3	1.60	0.83
1:A:1:MET:HB2	1:A:3:TYR:CE1	2.13	0.83
1:A:37:ILE:HD11	1:A:162:PHE:CZ	2.13	0.83
1:B:30:PHE:HB3	1:B:31:PRO:CD	2.09	0.82
1:A:34:LEU:HB3	1:A:40:ILE:HG21	1.61	0.82
1:A:48:ILE:HA	1:A:108:ILE:HG23	1.61	0.82
1:A:30:PHE:HB3	1:A:31:PRO:CD	2.09	0.82
1:B:275:ILE:HG21	1:B:327:PRO:HG3	1.60	0.82
1:B:22:ILE:HB	1:B:118:PHE:HZ	1.44	0.82
1:A:85:VAL:HG21	1:A:178:LEU:HD13	1.62	0.82
1:B:289:LYS:HE3	1:B:400:LEU:HB3	1.62	0.82
1:B:37:ILE:HD11	1:B:162:PHE:CZ	2.14	0.81
1:B:34:LEU:HB3	1:B:40:ILE:HG21	1.60	0.81
1:B:168:PHE:O	1:B:171:TRP:HB2	1.80	0.81
1:A:20:PHE:CD2	1:A:151:TRP:HB2	2.15	0.81
1:A:279:ALA:HB3	1:A:280:PRO:HD3	1.63	0.80
1:A:81:THR:O	1:A:85:VAL:HG23	1.81	0.80
1:B:90:PHE:CG	1:B:114:LEU:HD13	2.16	0.80
1:B:195:ALA:O	1:B:196:THR:HG22	1.81	0.80
1:A:163:THR:HG21	1:A:255:GLU:HA	1.65	0.79
1:B:20:PHE:CD2	1:B:151:TRP:HB2	2.17	0.79
1:B:163:THR:HG21	1:B:255:GLU:HA	1.65	0.79
1:B:88:ALA:HB3	1:B:89:PRO:HD3	1.65	0.78
1:A:85:VAL:HG22	1:A:178:LEU:HB2	1.66	0.78
1:A:166:ASN:OD1	1:A:167:GLN:N	2.15	0.78
1:B:1:MET:O	1:B:3:TYR:N	2.15	0.78
1:B:28:PRO:O	1:B:31:PRO:HD2	1.83	0.78
1:A:275:ILE:HG21	1:A:327:PRO:HG3	1.66	0.78
1:A:10:TRP:HE1	1:B:168:PHE:HD1	1.29	0.78
1:A:27:PHE:HB3	1:A:28:PRO:CD	2.13	0.78
1:A:121:GLY:HA2	1:A:124:ALA:HB3	1.65	0.78
1:B:37:ILE:HD13	1:B:166:ASN:HD22	1.48	0.78
1:B:41:SER:O	1:B:45:THR:HG23	1.84	0.78
1:A:251:PHE:CE2	1:A:260:VAL:HG21	2.19	0.78
1:B:85:VAL:HG21	1:B:178:LEU:HD13	1.65	0.77
1:A:74:LYS:HD2	1:A:74:LYS:N	1.97	0.77
1:A:28:PRO:O	1:A:31:PRO:HD2	1.84	0.77
1:B:22:ILE:HB	1:B:118:PHE:CZ	2.19	0.77
1:A:412:GLN:O	1:A:416:VAL:HG23	1.85	0.77
1:B:99:LEU:HD22	1:B:104:LEU:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PHE:HE1	1:B:129:ILE:HG21	1.50	0.76
1:B:48:ILE:HA	1:B:108:ILE:HG23	1.65	0.76
1:A:34:LEU:HB3	1:A:40:ILE:CG2	2.15	0.76
1:B:74:LYS:N	1:B:74:LYS:HD2	2.00	0.76
1:B:340:GLN:HE22	1:B:405:PRO:HB3	1.51	0.76
1:B:16:PHE:HB3	1:B:147:GLY:HA3	1.69	0.75
1:B:90:PHE:CE2	1:B:114:LEU:HB3	2.22	0.75
1:B:166:ASN:OD1	1:B:167:GLN:N	2.19	0.75
1:A:16:PHE:HB3	1:A:147:GLY:HA3	1.69	0.75
1:B:33:TRP:O	1:B:37:ILE:HB	1.85	0.75
1:B:34:LEU:HB3	1:B:40:ILE:CG2	2.15	0.75
1:B:412:GLN:O	1:B:416:VAL:HG23	1.86	0.75
1:B:251:PHE:CE2	1:B:260:VAL:HG21	2.22	0.75
1:B:85:VAL:HG22	1:B:178:LEU:HB2	1.69	0.75
1:A:1:MET:O	1:A:4:LEU:N	2.13	0.74
1:A:1:MET:O	1:A:3:TYR:N	2.20	0.74
1:A:195:ALA:O	1:A:196:THR:HG22	1.85	0.74
1:A:234:CYS:SG	1:A:365:MET:SD	2.82	0.74
1:A:1:MET:HB2	1:A:3:TYR:CZ	2.23	0.74
1:A:121:GLY:O	1:A:124:ALA:HB3	1.86	0.74
1:B:27:PHE:HB3	1:B:28:PRO:HD2	1.68	0.74
1:B:87:PHE:HB3	1:B:174:SER:HB2	1.69	0.74
1:B:99:LEU:CD2	1:B:104:LEU:HD12	2.16	0.74
1:B:271:LEU:HD23	1:B:323:MET:HB2	1.69	0.74
1:A:41:SER:O	1:A:45:THR:HG23	1.87	0.74
1:A:168:PHE:O	1:A:171:TRP:HB2	1.88	0.73
1:B:61:PRO:O	1:B:65:LEU:HG	1.88	0.73
1:B:246:PHE:CD1	1:B:246:PHE:C	2.62	0.73
1:A:44:ASP:HA	1:A:104:LEU:HD21	1.71	0.73
1:A:122:ALA:HB3	1:A:123:PRO:CD	2.18	0.73
1:A:10:TRP:HZ2	1:B:168:PHE:CE1	2.07	0.73
1:B:1:MET:HB2	1:B:3:TYR:CZ	2.23	0.73
1:B:74:LYS:HD2	1:B:74:LYS:H	1.53	0.73
1:A:172:LEU:HD13	1:B:183:LEU:HD12	1.71	0.72
1:B:230:ILE:HD11	1:B:357:PHE:HB3	1.71	0.72
1:A:22:ILE:HB	1:A:118:PHE:HZ	1.54	0.72
1:B:93:PHE:O	1:B:97:PRO:HG2	1.90	0.72
1:B:163:THR:HG21	1:B:255:GLU:HG3	1.71	0.72
1:B:171:TRP:HA	1:B:171:TRP:CE3	2.24	0.72
1:A:340:GLN:HE22	1:A:405:PRO:HB3	1.54	0.72
1:B:121:GLY:HA2	1:B:124:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:HB3	1:A:28:PRO:HD2	1.71	0.72
1:A:90:PHE:CE2	1:A:114:LEU:HB3	2.24	0.72
1:A:122:ALA:HB3	1:A:123:PRO:HD2	1.71	0.72
1:B:335:LYS:O	1:B:338:THR:HG22	1.89	0.72
1:A:87:PHE:HB3	1:A:174:SER:HB2	1.71	0.72
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.70	0.72
1:B:136:SER:O	1:B:137:ASN:CB	2.38	0.72
1:B:16:PHE:CE1	1:B:129:ILE:HG21	2.25	0.71
1:B:1:MET:O	1:B:4:LEU:N	2.17	0.71
1:B:215:GLU:O	1:B:218:ARG:HB3	1.90	0.71
1:B:122:ALA:HB3	1:B:123:PRO:CD	2.20	0.71
1:A:323:MET:O	1:A:327:PRO:HD2	1.91	0.71
1:A:165:ASN:O	1:A:168:PHE:HB3	1.89	0.71
1:A:338:THR:HG21	1:A:415:GLU:OE2	1.91	0.71
1:B:198:ALA:HB3	1:B:201:VAL:HG23	1.72	0.70
1:A:163:THR:HG21	1:A:255:GLU:HG3	1.73	0.70
1:A:16:PHE:HE1	1:A:129:ILE:HG21	1.56	0.70
1:B:246:PHE:HB2	1:B:378:PHE:CE2	2.26	0.70
1:A:289:LYS:HE3	1:A:400:LEU:HB3	1.73	0.70
1:A:44:ASP:OD1	1:A:104:LEU:HD22	1.92	0.70
1:B:122:ALA:HB3	1:B:123:PRO:HD2	1.74	0.69
1:B:216:LEU:HD23	1:B:219:GLN:OE1	1.92	0.69
1:B:338:THR:HG21	1:B:415:GLU:OE2	1.92	0.69
1:B:415:GLU:OE1	1:B:415:GLU:HA	1.91	0.69
1:A:335:LYS:O	1:A:338:THR:HG22	1.93	0.69
1:A:246:PHE:CD1	1:A:246:PHE:C	2.66	0.69
1:A:90:PHE:CZ	1:A:114:LEU:HB3	2.28	0.69
1:A:196:THR:CG2	1:A:201:VAL:HB	2.21	0.69
1:A:215:GLU:O	1:A:218:ARG:HB3	1.93	0.69
1:B:119:ASN:O	1:B:123:PRO:HD2	1.93	0.69
1:A:74:LYS:HD2	1:A:74:LYS:H	1.53	0.69
1:B:90:PHE:CZ	1:B:114:LEU:HB3	2.28	0.69
1:A:66:LEU:O	1:A:70:LEU:HG	1.92	0.69
1:A:22:ILE:HB	1:A:118:PHE:CZ	2.27	0.68
1:A:289:LYS:HA	1:A:400:LEU:HD21	1.74	0.68
1:B:333:CYS:O	1:B:337:ILE:HG13	1.93	0.68
1:B:121:GLY:O	1:B:124:ALA:HB3	1.94	0.68
1:B:16:PHE:CD1	1:B:129:ILE:HD12	2.28	0.68
1:B:171:TRP:HA	1:B:171:TRP:HE3	1.58	0.68
1:B:44:ASP:HA	1:B:104:LEU:HD21	1.75	0.68
1:A:243:PHE:O	1:A:246:PHE:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD11	1:A:357:PHE:HB3	1.75	0.68
1:A:33:TRP:O	1:A:37:ILE:HB	1.92	0.68
1:A:283:ILE:HG13	1:A:331:VAL:CG1	2.24	0.67
1:A:50:ALA:HB2	1:A:366:SER:CB	2.23	0.67
1:B:37:ILE:HD11	1:B:162:PHE:CE1	2.30	0.67
1:B:198:ALA:HB3	1:B:201:VAL:CG2	2.25	0.67
1:A:9:PHE:HD2	1:A:10:TRP:HE3	1.41	0.67
1:A:171:TRP:HA	1:A:171:TRP:CE3	2.29	0.67
1:A:172:LEU:HD13	1:B:183:LEU:CD1	2.25	0.67
1:A:307:SER:HA	1:A:379:GLN:NE2	2.09	0.67
1:B:16:PHE:CE1	1:B:129:ILE:HD12	2.30	0.67
1:A:216:LEU:HD23	1:A:219:GLN:OE1	1.95	0.66
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.30	0.66
1:A:276:MET:HA	1:A:279:ALA:HB2	1.76	0.66
1:A:37:ILE:HD11	1:A:162:PHE:CE1	2.29	0.66
1:A:108:ILE:HG22	1:A:112:ILE:HD11	1.76	0.66
1:A:119:ASN:O	1:A:123:PRO:HD2	1.94	0.66
1:A:9:PHE:CD2	1:A:10:TRP:HE3	2.14	0.66
1:A:136:SER:O	1:A:137:ASN:CB	2.43	0.66
1:A:4:LEU:HD22	1:A:10:TRP:HZ3	1.61	0.65
1:B:50:ALA:HB2	1:B:366:SER:CB	2.24	0.65
1:B:307:SER:HA	1:B:379:GLN:NE2	2.10	0.65
1:A:37:ILE:CD1	1:A:166:ASN:HD22	2.09	0.65
1:B:134:ARG:NH1	1:B:203:ALA:HA	2.12	0.65
1:A:271:LEU:HD23	1:A:323:MET:HB2	1.78	0.65
1:B:289:LYS:HA	1:B:400:LEU:HD21	1.77	0.65
1:A:90:PHE:CD2	1:A:114:LEU:HD22	2.32	0.65
1:B:196:THR:CG2	1:B:201:VAL:HB	2.24	0.65
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.32	0.65
1:A:48:ILE:HA	1:A:108:ILE:CG2	2.27	0.65
1:A:289:LYS:HD3	1:A:403:PRO:HG3	1.77	0.65
1:B:323:MET:SD	1:B:323:MET:N	2.70	0.65
1:A:10:TRP:HB3	1:A:11:MET:HE3	1.80	0.64
1:A:158:VAL:O	1:A:162:PHE:N	2.22	0.64
1:A:177:ALA:O	1:A:181:ALA:HB2	1.97	0.64
1:B:237:ASP:O	1:B:238:VAL:C	2.35	0.64
1:A:7:THR:O	1:A:11:MET:HG2	1.98	0.64
1:A:42:LYS:HZ2	1:A:373:TYR:HB3	1.62	0.64
1:A:49:PHE:HB3	1:A:241:GLN:OE1	1.96	0.64
1:A:61:PRO:O	1:A:65:LEU:HG	1.98	0.64
1:A:99:LEU:CD2	1:A:104:LEU:HD12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:CA	1:A:124:ALA:HB3	2.27	0.64
1:B:90:PHE:CD2	1:B:114:LEU:HD22	2.32	0.64
1:B:282:ILE:O	1:B:286:ILE:HG13	1.98	0.64
1:A:26:TYR:CD1	1:A:27:PHE:N	2.66	0.64
1:B:108:ILE:O	1:B:111:GLY:N	2.29	0.64
1:B:29:PHE:CE1	1:B:33:TRP:CD1	2.86	0.64
1:B:283:ILE:HG13	1:B:331:VAL:CG1	2.27	0.63
1:B:292:LEU:HD21	1:B:333:CYS:N	2.13	0.63
1:A:99:LEU:HD22	1:A:104:LEU:HD12	1.81	0.63
1:A:108:ILE:O	1:A:111:GLY:N	2.32	0.63
1:A:196:THR:HG21	1:A:201:VAL:CB	2.26	0.63
1:B:127:ALA:O	1:B:130:GLU:N	2.31	0.63
1:A:32:ILE:HD13	1:A:258:THR:HG23	1.79	0.63
1:A:307:SER:HA	1:A:379:GLN:HE21	1.63	0.63
1:B:16:PHE:HB3	1:B:147:GLY:CA	2.29	0.63
1:B:161:MET:HB3	1:B:168:PHE:HE2	1.64	0.63
1:A:34:LEU:HD13	1:A:40:ILE:CD1	2.24	0.63
1:A:16:PHE:HB3	1:A:147:GLY:CA	2.29	0.62
1:A:16:PHE:CD1	1:A:129:ILE:HD12	2.34	0.62
1:A:279:ALA:O	1:A:283:ILE:HG12	1.98	0.62
1:A:133:SER:HG	1:A:138:PHE:C	2.02	0.62
1:A:292:LEU:HD21	1:A:333:CYS:N	2.14	0.62
1:A:319:LYS:O	1:A:320:THR:C	2.38	0.62
1:B:76:LEU:HA	1:B:79:ILE:HD12	1.80	0.62
1:A:239:PHE:CE2	1:A:303:ILE:HG12	2.34	0.62
1:B:107:SER:O	1:B:111:GLY:N	2.32	0.62
1:A:171:TRP:HA	1:A:171:TRP:HE3	1.65	0.62
1:B:90:PHE:CE2	1:B:95:PHE:HE1	2.18	0.62
1:B:323:MET:O	1:B:327:PRO:HD2	1.99	0.62
1:A:85:VAL:HG13	1:A:178:LEU:HB2	1.81	0.62
1:B:108:ILE:HG22	1:B:112:ILE:HD11	1.81	0.62
1:A:29:PHE:CE1	1:A:33:TRP:CD1	2.87	0.62
1:B:278:PHE:O	1:B:282:ILE:HG13	2.00	0.62
1:B:379:GLN:O	1:B:382:TYR:HB2	1.99	0.62
1:B:161:MET:HB3	1:B:168:PHE:CE2	2.35	0.62
1:A:16:PHE:CE1	1:A:129:ILE:HD12	2.35	0.62
1:B:277:PHE:C	1:B:278:PHE:HD1	2.03	0.62
1:B:63:PHE:CE1	1:B:124:ALA:HB2	2.35	0.61
1:A:237:ASP:O	1:A:238:VAL:C	2.38	0.61
1:A:283:ILE:O	1:A:287:GLY:N	2.33	0.61
1:B:76:LEU:HD12	1:B:79:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:HB3	1:B:151:TRP:HB2	1.82	0.61
1:B:340:GLN:NE2	1:B:405:PRO:HB3	2.13	0.61
1:B:411:ARG:O	1:B:414:ASN:HB3	2.00	0.61
1:A:289:LYS:HG3	1:A:400:LEU:CD2	2.19	0.61
1:B:52:ILE:N	1:B:112:ILE:HD13	2.16	0.61
1:B:177:ALA:O	1:B:181:ALA:HB2	2.00	0.61
1:B:243:PHE:O	1:B:246:PHE:HB3	2.01	0.61
1:B:12:PHE:HE2	1:B:132:VAL:HG21	1.66	0.61
1:A:323:MET:SD	1:A:323:MET:N	2.73	0.61
1:B:246:PHE:HD1	1:B:247:PHE:N	1.99	0.61
1:B:44:ASP:OD1	1:B:104:LEU:HD22	2.01	0.61
1:B:289:LYS:HD3	1:B:403:PRO:HG3	1.81	0.61
1:A:42:LYS:HG3	1:A:374:GLU:N	2.16	0.60
1:B:163:THR:CG2	1:B:255:GLU:HG3	2.31	0.60
1:B:368:LEU:O	1:B:372:MET:HG3	2.01	0.60
1:A:337:ILE:CD1	1:A:350:TYR:HE1	2.14	0.60
1:B:10:TRP:HB3	1:B:11:MET:HE3	1.83	0.60
1:B:326:VAL:O	1:B:327:PRO:C	2.39	0.60
1:B:329:LEU:O	1:B:333:CYS:HB2	2.00	0.60
1:A:239:PHE:HD1	1:A:240:ASP:N	1.99	0.60
1:A:77:LEU:O	1:A:80:ILE:HB	2.01	0.60
1:A:264:VAL:O	1:A:265:THR:C	2.40	0.60
1:B:307:SER:HA	1:B:379:GLN:HE21	1.66	0.60
1:A:40:ILE:HD13	1:A:45:THR:HG22	1.83	0.60
1:A:107:SER:O	1:A:111:GLY:N	2.35	0.60
1:A:277:PHE:C	1:A:278:PHE:HD1	2.05	0.60
1:A:283:ILE:HG13	1:A:331:VAL:HG11	1.82	0.60
1:B:4:LEU:HD22	1:B:10:TRP:HZ3	1.66	0.60
1:B:9:PHE:CD2	1:B:10:TRP:HE3	2.20	0.60
1:B:165:ASN:O	1:B:168:PHE:HB3	2.02	0.60
1:B:49:PHE:HB3	1:B:241:GLN:OE1	2.01	0.60
1:B:95:PHE:O	1:B:96:GLY:C	2.40	0.60
1:B:279:ALA:O	1:B:283:ILE:HG12	2.01	0.60
1:A:20:PHE:HB3	1:A:151:TRP:HB2	1.83	0.59
1:A:340:GLN:NE2	1:A:405:PRO:HB3	2.17	0.59
1:A:368:LEU:O	1:A:372:MET:HG3	2.02	0.59
1:A:198:ALA:HB3	1:A:201:VAL:HG23	1.84	0.59
1:B:66:LEU:O	1:B:70:LEU:HG	2.01	0.59
1:B:338:THR:CG2	1:B:339:SER:N	2.64	0.59
1:A:98:LEU:HB2	1:A:107:SER:OG	2.03	0.59
1:A:163:THR:CG2	1:A:255:GLU:HG3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:MET:HA	1:A:326:VAL:HG23	1.84	0.59
1:A:338:THR:CG2	1:A:339:SER:N	2.64	0.59
1:A:20:PHE:HD1	1:A:20:PHE:H	1.50	0.59
1:A:246:PHE:HD1	1:A:247:PHE:N	2.01	0.59
1:B:9:PHE:HD2	1:B:10:TRP:HE3	1.49	0.59
1:B:239:PHE:CD1	1:B:239:PHE:C	2.75	0.59
1:A:52:ILE:N	1:A:112:ILE:HD13	2.18	0.59
1:A:415:GLU:HA	1:A:415:GLU:OE1	2.03	0.59
1:B:283:ILE:HG13	1:B:331:VAL:HG11	1.84	0.59
1:B:348:THR:HA	1:B:351:LEU:HD12	1.85	0.59
1:B:50:ALA:O	1:B:53:SER:HB3	2.03	0.59
1:B:224:PHE:CD2	1:B:399:THR:CG2	2.86	0.59
1:B:225:LEU:HD13	1:B:336:TYR:CE2	2.38	0.59
1:B:239:PHE:HD1	1:B:240:ASP:N	1.99	0.59
1:A:63:PHE:CE1	1:A:124:ALA:HB2	2.38	0.59
1:B:276:MET:HA	1:B:279:ALA:HB2	1.83	0.59
1:B:85:VAL:HG13	1:B:178:LEU:HB2	1.85	0.58
1:B:158:VAL:O	1:B:162:PHE:N	2.30	0.58
1:B:40:ILE:HG12	1:B:45:THR:HG23	1.85	0.58
1:B:90:PHE:O	1:B:94:ILE:HG13	2.02	0.58
1:B:196:THR:HG21	1:B:201:VAL:CB	2.30	0.58
1:B:253:THR:HG22	1:B:254:GLY:N	2.17	0.58
1:A:90:PHE:CE2	1:A:95:PHE:HE1	2.20	0.58
1:A:239:PHE:HE2	1:A:303:ILE:HA	1.68	0.58
1:A:373:TYR:HE1	1:A:382:TYR:HE1	1.51	0.58
1:B:90:PHE:HD1	1:B:94:ILE:HD12	1.67	0.58
1:A:62:LEU:O	1:A:66:LEU:HG	2.03	0.58
1:A:76:LEU:HA	1:A:79:ILE:HD12	1.84	0.58
1:B:264:VAL:O	1:B:265:THR:C	2.42	0.58
1:A:4:LEU:HD22	1:A:10:TRP:CZ3	2.37	0.58
1:A:348:THR:HA	1:A:351:LEU:HD12	1.85	0.58
1:B:294:LEU:O	1:B:298:ILE:HG13	2.03	0.58
1:A:410:ARG:O	1:A:413:VAL:HB	2.04	0.58
1:A:127:ALA:O	1:A:130:GLU:N	2.36	0.58
1:A:289:LYS:HA	1:A:400:LEU:CD2	2.34	0.58
1:B:390:LEU:C	1:B:390:LEU:HD23	2.24	0.58
1:A:172:LEU:CD1	1:B:183:LEU:HD12	2.33	0.58
1:A:282:ILE:O	1:A:286:ILE:HG13	2.04	0.58
1:B:20:PHE:HD1	1:B:20:PHE:H	1.52	0.58
1:B:121:GLY:CA	1:B:124:ALA:HB3	2.34	0.58
1:B:347:ALA:O	1:B:351:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HH21	1:A:192:PRO:HA	1.69	0.58
1:A:326:VAL:HB	1:A:327:PRO:HD3	1.85	0.58
1:A:347:ALA:O	1:A:351:LEU:HG	2.04	0.58
1:B:307:SER:C	1:B:379:GLN:NE2	2.57	0.58
1:B:26:TYR:CD2	1:B:27:PHE:N	2.72	0.57
1:A:50:ALA:HB1	1:A:363:ILE:HA	1.86	0.57
1:B:37:ILE:HD11	1:B:162:PHE:HZ	1.67	0.57
1:A:10:TRP:CZ2	1:B:168:PHE:CE1	2.92	0.57
1:A:154:GLY:O	1:A:155:ALA:C	2.43	0.57
1:B:283:ILE:O	1:B:287:GLY:N	2.37	0.57
1:B:346:SER:OG	1:B:347:ALA:N	2.36	0.57
1:A:42:LYS:NZ	1:A:373:TYR:HB3	2.17	0.57
1:B:16:PHE:HE1	1:B:129:ILE:CG2	2.17	0.57
1:B:225:LEU:HD13	1:B:336:TYR:HE2	1.69	0.57
1:A:134:ARG:NH1	1:A:203:ALA:HA	2.18	0.57
1:B:29:PHE:HE1	1:B:33:TRP:CD1	2.23	0.57
1:B:42:LYS:HG3	1:B:374:GLU:N	2.20	0.57
1:B:55:PHE:O	1:B:59:PHE:HB2	2.04	0.57
1:B:148:CYS:O	1:B:148:CYS:SG	2.63	0.57
1:B:278:PHE:N	1:B:278:PHE:CD1	2.73	0.57
1:A:74:LYS:H	1:A:74:LYS:CD	2.15	0.57
1:A:127:ALA:O	1:A:128:PHE:C	2.43	0.57
1:A:133:SER:OG	1:A:139:GLU:HA	2.05	0.57
1:B:133:SER:OG	1:B:139:GLU:HA	2.05	0.57
1:A:263:TYR:HD1	1:A:263:TYR:H	1.53	0.57
1:B:337:ILE:CD1	1:B:350:TYR:HE1	2.18	0.57
1:A:121:GLY:C	1:A:124:ALA:HB3	2.26	0.56
1:A:78:TRP:C	1:A:80:ILE:N	2.58	0.56
1:A:49:PHE:O	1:A:52:ILE:HB	2.04	0.56
1:A:93:PHE:O	1:A:97:PRO:HG2	2.04	0.56
1:A:113:TYR:C	1:A:115:GLY:N	2.55	0.56
1:A:253:THR:HG22	1:A:254:GLY:N	2.21	0.56
1:A:18:PHE:CE1	1:A:180:LEU:HD12	2.41	0.56
1:B:263:TYR:HD1	1:B:263:TYR:H	1.53	0.56
1:B:326:VAL:HB	1:B:327:PRO:HD2	1.83	0.56
1:A:25:ALA:HA	1:A:158:VAL:HG21	1.88	0.56
1:A:239:PHE:CD1	1:A:239:PHE:C	2.78	0.56
1:A:333:CYS:O	1:A:337:ILE:HG13	2.05	0.56
1:B:208:PHE:HA	1:B:212:LEU:HD12	1.88	0.56
1:A:37:ILE:HD11	1:A:162:PHE:HZ	1.65	0.56
1:A:90:PHE:CB	1:A:114:LEU:HD13	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:HB3	1:A:201:VAL:CG2	2.36	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CD2	2.24	0.56
1:B:48:ILE:HA	1:B:108:ILE:CG2	2.32	0.56
1:B:278:PHE:HD1	1:B:278:PHE:N	2.03	0.56
1:A:2:TYR:CE1	1:A:137:ASN:ND2	2.74	0.56
1:A:108:ILE:O	1:A:112:ILE:HG13	2.05	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CE2	2.24	0.56
1:B:44:ASP:O	1:B:48:ILE:HG13	2.06	0.56
1:B:74:LYS:H	1:B:74:LYS:CD	2.16	0.56
1:B:13:GLY:O	1:B:146:PHE:HD2	1.89	0.56
1:B:2:TYR:CE1	1:B:137:ASN:ND2	2.74	0.56
1:B:212:LEU:HD22	1:B:345:PHE:CE1	2.40	0.56
1:A:63:PHE:CE2	1:A:76:LEU:HD21	2.41	0.55
1:B:239:PHE:C	1:B:239:PHE:HD1	2.09	0.55
1:A:12:PHE:O	1:A:15:PHE:N	2.39	0.55
1:A:44:ASP:HA	1:A:104:LEU:CD2	2.36	0.55
1:A:208:PHE:HA	1:A:212:LEU:HD12	1.88	0.55
1:A:338:THR:HG23	1:A:339:SER:N	2.21	0.55
1:B:50:ALA:HB1	1:B:363:ILE:HA	1.89	0.55
1:B:85:VAL:CG2	1:B:178:LEU:HD13	2.36	0.55
1:B:116:PHE:C	1:B:118:PHE:H	2.10	0.55
1:A:12:PHE:HE2	1:A:132:VAL:HG21	1.72	0.55
1:A:85:VAL:HG21	1:A:178:LEU:CD1	2.34	0.55
1:B:271:LEU:HD23	1:B:323:MET:CB	2.35	0.55
1:A:278:PHE:O	1:A:282:ILE:HG13	2.06	0.55
1:B:34:LEU:CB	1:B:40:ILE:HG21	2.36	0.55
1:B:98:LEU:HB2	1:B:107:SER:OG	2.06	0.55
1:A:24:GLY:O	1:A:25:ALA:C	2.45	0.55
1:A:215:GLU:OE1	1:A:215:GLU:C	2.45	0.55
1:B:25:ALA:HA	1:B:158:VAL:HG21	1.89	0.55
1:B:289:LYS:HA	1:B:400:LEU:CD2	2.35	0.55
1:A:296:GLY:HA2	1:A:299:MET:HE3	1.88	0.55
1:B:18:PHE:CE1	1:B:180:LEU:HD12	2.41	0.55
1:A:224:PHE:CD1	1:A:224:PHE:N	2.72	0.55
1:A:17:PHE:HD2	1:A:18:PHE:CE2	2.25	0.55
1:A:85:VAL:CG2	1:A:178:LEU:HD13	2.35	0.55
1:B:136:SER:O	1:B:137:ASN:HB2	2.06	0.55
1:A:228:TYR:CZ	1:A:292:LEU:HB3	2.42	0.55
1:A:346:SER:OG	1:A:347:ALA:N	2.40	0.55
1:B:44:ASP:HA	1:B:104:LEU:CD2	2.36	0.55
1:B:47:ILE:O	1:B:48:ILE:C	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:O	1:B:282:ILE:HB	2.07	0.55
1:A:29:PHE:HE1	1:A:33:TRP:CD1	2.25	0.54
1:A:121:GLY:HA2	1:A:124:ALA:CB	2.34	0.54
1:B:27:PHE:CB	1:B:28:PRO:CD	2.83	0.54
1:B:236:TYR:HH	1:B:322:HIS:HD1	1.51	0.54
1:B:127:ALA:O	1:B:130:GLU:HB3	2.08	0.54
1:B:275:ILE:HG21	1:B:327:PRO:CG	2.35	0.54
1:A:20:PHE:HB3	1:A:151:TRP:CA	2.37	0.54
1:A:326:VAL:O	1:A:327:PRO:C	2.45	0.54
1:B:124:ALA:O	1:B:127:ALA:N	2.39	0.54
1:A:55:PHE:O	1:A:59:PHE:HB2	2.07	0.54
1:A:311:SER:O	1:A:314:GLU:HB3	2.07	0.54
1:B:135:ARG:HH21	1:B:192:PRO:HA	1.71	0.54
1:A:283:ILE:HG13	1:A:331:VAL:HG12	1.90	0.54
1:A:336:TYR:OH	1:A:401:SER:HB2	2.07	0.54
1:B:108:ILE:O	1:B:109:VAL:C	2.46	0.54
1:B:135:ARG:O	1:B:135:ARG:HD3	2.08	0.54
1:B:151:TRP:CD1	1:B:269:GLU:HG3	2.42	0.54
1:B:338:THR:HG23	1:B:339:SER:N	2.22	0.54
1:A:78:TRP:C	1:A:80:ILE:H	2.11	0.54
1:A:336:TYR:OH	1:A:401:SER:CB	2.56	0.54
1:B:307:SER:CA	1:B:379:GLN:NE2	2.71	0.54
1:B:33:TRP:CD1	1:B:37:ILE:HD13	2.43	0.54
1:B:246:PHE:C	1:B:246:PHE:HD1	2.09	0.54
1:A:13:GLY:O	1:A:146:PHE:HD2	1.91	0.54
1:B:40:ILE:HD13	1:B:45:THR:HG22	1.90	0.54
1:B:42:LYS:HZ2	1:B:373:TYR:HB3	1.73	0.54
1:A:10:TRP:NE1	1:B:168:PHE:HD1	2.03	0.53
1:A:55:PHE:CZ	1:A:113:TYR:HE1	2.27	0.53
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.90	0.53
1:A:307:SER:C	1:A:379:GLN:NE2	2.61	0.53
1:B:24:GLY:O	1:B:25:ALA:C	2.44	0.53
1:A:47:ILE:O	1:A:48:ILE:C	2.47	0.53
1:A:239:PHE:HD1	1:A:239:PHE:C	2.12	0.53
1:B:20:PHE:HB3	1:B:151:TRP:CA	2.38	0.53
1:B:125:VAL:O	1:B:129:ILE:HG13	2.08	0.53
1:B:113:TYR:O	1:B:116:PHE:HD2	1.91	0.53
1:B:275:ILE:CG2	1:B:327:PRO:HG3	2.35	0.53
1:A:141:GLY:O	1:A:145:MET:HG3	2.08	0.53
1:B:133:SER:HG	1:B:138:PHE:C	2.12	0.53
1:B:141:GLY:O	1:B:145:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:C	1:B:215:GLU:OE1	2.47	0.53
1:A:225:LEU:HD13	1:A:336:TYR:CE2	2.44	0.53
1:B:7:THR:O	1:B:11:MET:HG2	2.08	0.53
1:B:319:LYS:O	1:B:320:THR:C	2.46	0.53
1:A:278:PHE:N	1:A:278:PHE:CD1	2.77	0.53
1:A:307:SER:CA	1:A:379:GLN:NE2	2.71	0.53
1:B:28:PRO:O	1:B:29:PHE:C	2.46	0.53
1:A:277:PHE:HD2	1:A:278:PHE:CE1	2.27	0.53
1:A:326:VAL:HB	1:A:327:PRO:HD2	1.87	0.53
1:B:49:PHE:O	1:B:52:ILE:HB	2.08	0.53
1:B:33:TRP:HD1	1:B:37:ILE:HD13	1.74	0.53
1:A:90:PHE:O	1:A:94:ILE:HG13	2.09	0.53
1:A:174:SER:O	1:A:177:ALA:HB3	2.09	0.53
1:B:1:MET:O	1:B:2:TYR:C	2.47	0.53
1:B:42:LYS:NZ	1:B:378:PHE:CE1	2.77	0.53
1:B:112:ILE:O	1:B:112:ILE:HG22	2.09	0.53
1:B:319:LYS:O	1:B:322:HIS:N	2.31	0.53
1:A:17:PHE:HD2	1:A:18:PHE:CD2	2.27	0.53
1:A:85:VAL:CG2	1:A:178:LEU:HB2	2.38	0.53
1:A:244:ALA:O	1:A:247:PHE:N	2.42	0.53
1:B:277:PHE:HD2	1:B:278:PHE:CE1	2.27	0.53
1:A:95:PHE:O	1:A:96:GLY:C	2.46	0.52
1:A:289:LYS:O	1:A:293:LEU:HG	2.09	0.52
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.39	0.52
1:B:299:MET:SD	1:B:325:GLU:OE2	2.66	0.52
1:A:116:PHE:C	1:A:118:PHE:H	2.12	0.52
1:B:116:PHE:O	1:B:118:PHE:N	2.42	0.52
1:A:116:PHE:O	1:A:118:PHE:N	2.42	0.52
1:A:135:ARG:O	1:A:135:ARG:HD3	2.10	0.52
1:B:224:PHE:CD1	1:B:224:PHE:N	2.76	0.52
1:B:239:PHE:HE2	1:B:303:ILE:HA	1.73	0.52
1:A:112:ILE:HG22	1:A:112:ILE:O	2.10	0.52
1:A:107:SER:O	1:A:111:GLY:HA3	2.08	0.52
1:A:226:SER:O	1:A:227:LEU:C	2.48	0.52
1:A:246:PHE:C	1:A:246:PHE:HD1	2.13	0.52
1:B:12:PHE:O	1:B:15:PHE:N	2.42	0.52
1:B:77:LEU:O	1:B:80:ILE:HB	2.10	0.52
1:B:78:TRP:C	1:B:80:ILE:N	2.63	0.52
1:B:151:TRP:HD1	1:B:269:GLU:HG3	1.73	0.52
1:B:303:ILE:HG21	1:B:386:GLY:CA	2.39	0.52
1:B:373:TYR:HE1	1:B:382:TYR:HE1	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:O	1:A:414:ASN:HB3	2.10	0.52
1:B:86:MET:O	1:B:89:PRO:HD2	2.10	0.52
1:A:263:TYR:CD1	1:A:263:TYR:N	2.77	0.52
1:A:278:PHE:HD1	1:A:278:PHE:N	2.08	0.52
1:B:228:TYR:CZ	1:B:292:LEU:HB3	2.45	0.52
1:A:382:TYR:O	1:A:383:LEU:C	2.46	0.52
1:B:289:LYS:HD2	1:B:401:SER:O	2.10	0.52
1:B:336:TYR:OH	1:B:401:SER:HB2	2.10	0.52
1:A:62:LEU:O	1:A:62:LEU:HD12	2.10	0.52
1:A:76:LEU:HD12	1:A:79:ILE:HD12	1.91	0.52
1:A:101:TYR:O	1:A:102:ASN:HB2	2.09	0.52
1:A:151:TRP:HD1	1:A:269:GLU:HG3	1.75	0.52
1:A:271:LEU:HG	1:A:275:ILE:HD11	1.92	0.52
1:A:289:LYS:HD2	1:A:401:SER:O	2.09	0.52
1:A:319:LYS:O	1:A:321:LEU:N	2.43	0.52
1:B:62:LEU:HD12	1:B:62:LEU:O	2.10	0.52
1:A:151:TRP:CD1	1:A:269:GLU:HG3	2.45	0.51
1:A:289:LYS:CG	1:A:400:LEU:HD23	2.23	0.51
1:B:113:TYR:C	1:B:115:GLY:N	2.61	0.51
1:B:179:ILE:O	1:B:183:LEU:HB2	2.10	0.51
1:B:263:TYR:N	1:B:263:TYR:CD1	2.77	0.51
1:B:336:TYR:OH	1:B:401:SER:CB	2.58	0.51
1:A:33:TRP:HD1	1:A:37:ILE:HD13	1.75	0.51
1:A:50:ALA:O	1:A:53:SER:HB3	2.10	0.51
1:A:136:SER:O	1:A:137:ASN:HB2	2.10	0.51
1:B:239:PHE:CE2	1:B:303:ILE:HG12	2.45	0.51
1:A:1:MET:SD	1:A:3:TYR:OH	2.58	0.51
1:A:9:PHE:CD2	1:A:10:TRP:CE3	2.98	0.51
1:A:18:PHE:CZ	1:A:180:LEU:CD1	2.94	0.51
1:A:70:LEU:HD11	1:A:76:LEU:HB2	1.92	0.51
1:A:127:ALA:O	1:A:130:GLU:HB3	2.11	0.51
1:B:34:LEU:HD13	1:B:40:ILE:CD1	2.36	0.51
1:B:226:SER:O	1:B:227:LEU:C	2.49	0.51
1:A:178:LEU:HG	1:A:179:ILE:N	2.26	0.51
1:A:33:TRP:HH2	1:A:95:PHE:HB2	1.76	0.51
1:A:135:ARG:NH2	1:A:192:PRO:HA	2.26	0.51
1:B:8:ASN:ND2	1:B:189:THR:OG1	2.44	0.51
1:B:40:ILE:HG13	1:B:44:ASP:HB2	1.92	0.51
1:A:33:TRP:CD1	1:A:37:ILE:HD13	2.45	0.51
1:A:40:ILE:HG12	1:A:45:THR:HG23	1.92	0.51
1:A:85:VAL:HG22	1:A:178:LEU:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:MET:HA	1:A:326:VAL:CG2	2.40	0.51
1:A:332:GLY:O	1:A:333:CYS:C	2.49	0.51
1:B:382:TYR:O	1:B:383:LEU:C	2.48	0.51
1:A:42:LYS:NZ	1:A:378:PHE:CE1	2.76	0.51
1:B:127:ALA:O	1:B:128:PHE:C	2.45	0.51
1:B:135:ARG:NH2	1:B:192:PRO:HA	2.26	0.51
1:A:1:MET:O	1:A:2:TYR:C	2.49	0.51
1:A:225:LEU:HD13	1:A:336:TYR:HE2	1.76	0.51
1:A:290:ASN:O	1:A:291:ALA:C	2.48	0.51
1:A:78:TRP:O	1:A:80:ILE:N	2.43	0.51
1:A:224:PHE:CD2	1:A:399:THR:CG2	2.94	0.51
1:A:390:LEU:C	1:A:390:LEU:HD23	2.32	0.51
1:B:236:TYR:CG	1:B:299:MET:SD	3.04	0.51
1:A:34:LEU:CB	1:A:40:ILE:HG21	2.38	0.50
1:B:320:THR:O	1:B:322:HIS:N	2.44	0.50
1:A:228:TYR:OH	1:A:292:LEU:O	2.29	0.50
1:A:279:ALA:O	1:A:282:ILE:HB	2.11	0.50
1:B:288:GLY:O	1:B:289:LYS:C	2.49	0.50
1:A:40:ILE:HG13	1:A:44:ASP:HB2	1.93	0.50
1:A:113:TYR:O	1:A:116:PHE:HD2	1.94	0.50
1:A:128:PHE:C	1:A:128:PHE:CD1	2.85	0.50
1:A:236:TYR:HH	1:A:322:HIS:HD1	1.56	0.50
1:A:315:VAL:O	1:A:316:VAL:C	2.49	0.50
1:A:294:LEU:O	1:A:298:ILE:HG13	2.11	0.50
1:B:277:PHE:HB3	1:B:278:PHE:CD1	2.47	0.50
1:B:323:MET:HA	1:B:326:VAL:HG23	1.94	0.50
1:A:173:GLY:O	1:A:177:ALA:HB2	2.12	0.50
1:B:29:PHE:CE1	1:B:170:PHE:CZ	3.00	0.50
1:B:38:ASN:HB3	1:B:100:GLN:NE2	2.27	0.50
1:B:104:LEU:O	1:B:108:ILE:HG13	2.12	0.50
1:B:289:LYS:HG3	1:B:400:LEU:CD2	2.23	0.50
1:B:303:ILE:O	1:B:306:SER:N	2.41	0.50
1:A:28:PRO:O	1:A:29:PHE:C	2.49	0.50
1:A:29:PHE:CD1	1:A:33:TRP:HB2	2.47	0.50
1:A:244:ALA:O	1:A:245:ASN:C	2.50	0.50
1:A:370:GLY:O	1:A:373:TYR:HB2	2.11	0.50
1:B:17:PHE:CD2	1:B:18:PHE:CE2	3.00	0.50
1:B:116:PHE:CG	1:B:117:CYS:N	2.79	0.50
1:A:9:PHE:O	1:A:10:TRP:C	2.50	0.49
1:A:336:TYR:CE2	1:A:400:LEU:HD11	2.47	0.49
1:B:4:LEU:HD22	1:B:10:TRP:CZ3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASN:O	1:B:291:ALA:C	2.50	0.49
1:B:370:GLY:O	1:B:373:TYR:HB2	2.11	0.49
1:B:55:PHE:CZ	1:B:113:TYR:HE1	2.30	0.49
1:B:116:PHE:C	1:B:116:PHE:CD1	2.85	0.49
1:B:400:LEU:HG	1:B:401:SER:N	2.27	0.49
1:A:121:GLY:O	1:A:125:VAL:N	2.43	0.49
1:A:161:MET:HB3	1:A:168:PHE:CE2	2.48	0.49
1:A:238:VAL:HA	1:A:241:GLN:NE2	2.27	0.49
1:A:288:GLY:O	1:A:289:LYS:C	2.48	0.49
1:B:76:LEU:CD1	1:B:79:ILE:HD12	2.42	0.49
1:B:86:MET:C	1:B:89:PRO:HD2	2.32	0.49
1:B:90:PHE:CB	1:B:114:LEU:HD13	2.41	0.49
1:A:124:ALA:O	1:A:127:ALA:N	2.45	0.49
1:A:381:ALA:O	1:A:384:VAL:N	2.46	0.49
1:A:34:LEU:HD22	1:A:40:ILE:HD12	1.95	0.49
1:B:121:GLY:C	1:B:124:ALA:HB3	2.33	0.49
1:A:25:ALA:O	1:A:26:TYR:C	2.50	0.49
1:A:161:MET:HB3	1:A:168:PHE:HE2	1.78	0.49
1:B:99:LEU:HD23	1:B:104:LEU:HA	1.95	0.49
1:B:101:TYR:O	1:B:102:ASN:HB2	2.13	0.49
1:B:230:ILE:O	1:B:234:CYS:HB2	2.13	0.49
1:A:29:PHE:CE1	1:A:170:PHE:CZ	3.01	0.49
1:A:45:THR:OG1	1:A:46:GLY:N	2.44	0.49
1:B:407:SER:OG	1:B:410:ARG:HB2	2.13	0.49
1:A:224:PHE:N	1:A:224:PHE:HD1	2.09	0.49
1:B:51:ALA:O	1:B:54:LEU:N	2.46	0.49
1:B:289:LYS:O	1:B:293:LEU:HG	2.13	0.49
1:B:246:PHE:HB2	1:B:378:PHE:HD2	1.70	0.48
1:A:99:LEU:HG	1:A:107:SER:OG	2.12	0.48
1:A:108:ILE:O	1:A:109:VAL:C	2.49	0.48
1:A:157:ILE:HG23	1:A:161:MET:HG3	1.94	0.48
1:A:312:ALA:HA	1:A:315:VAL:HG23	1.95	0.48
1:B:29:PHE:CD1	1:B:33:TRP:HB2	2.48	0.48
1:B:407:SER:HG	1:B:410:ARG:HB2	1.79	0.48
1:A:122:ALA:CB	1:A:123:PRO:CD	2.90	0.48
1:A:275:ILE:HG21	1:A:327:PRO:CG	2.39	0.48
1:A:405:PRO:O	1:A:407:SER:N	2.47	0.48
1:B:22:ILE:HD11	1:B:177:ALA:HB1	1.94	0.48
1:B:336:TYR:CZ	1:B:400:LEU:HD11	2.49	0.48
1:B:37:ILE:CD1	1:B:166:ASN:HD22	2.21	0.48
1:B:341:PHE:CD2	1:B:349:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD21	1:A:117:CYS:HB3	1.95	0.48
1:A:91:PHE:HB3	1:A:170:PHE:CE2	2.47	0.48
1:A:97:PRO:O	1:A:98:LEU:C	2.52	0.48
1:A:116:PHE:CG	1:A:117:CYS:N	2.81	0.48
1:A:320:THR:O	1:A:322:HIS:N	2.46	0.48
1:A:336:TYR:CZ	1:A:400:LEU:HD11	2.48	0.48
1:A:366:SER:O	1:A:369:ALA:HB3	2.13	0.48
1:B:62:LEU:O	1:B:66:LEU:HG	2.13	0.48
1:A:44:ASP:O	1:A:48:ILE:HG13	2.14	0.48
1:B:244:ALA:O	1:B:245:ASN:C	2.52	0.48
1:B:283:ILE:HG13	1:B:331:VAL:HG12	1.93	0.48
1:A:22:ILE:HD11	1:A:177:ALA:HB1	1.96	0.48
1:A:93:PHE:N	1:A:93:PHE:CD1	2.81	0.48
1:B:42:LYS:NZ	1:B:373:TYR:HB3	2.27	0.48
1:A:369:ALA:O	1:A:370:GLY:C	2.52	0.48
1:B:121:GLY:HA2	1:B:124:ALA:CB	2.43	0.48
1:A:1:MET:HA	1:A:5:LYS:HE3	1.96	0.48
1:A:55:PHE:CZ	1:A:113:TYR:CE1	3.02	0.48
1:A:239:PHE:CD1	1:A:240:ASP:N	2.82	0.48
1:A:305:GLY:O	1:A:318:LEU:HD11	2.13	0.48
1:A:329:LEU:O	1:A:333:CYS:HB2	2.14	0.48
1:A:104:LEU:HG	1:A:108:ILE:HD11	1.95	0.48
1:A:213:ALA:O	1:A:216:LEU:N	2.47	0.48
1:A:239:PHE:CD2	1:A:303:ILE:HG12	2.49	0.48
1:A:373:TYR:HE1	1:A:382:TYR:CE1	2.32	0.48
1:B:25:ALA:O	1:B:26:TYR:C	2.52	0.48
1:B:33:TRP:HH2	1:B:95:PHE:HB2	1.79	0.48
1:B:40:ILE:HG12	1:B:41:SER:O	2.14	0.48
1:B:128:PHE:C	1:B:128:PHE:CD1	2.85	0.48
1:A:90:PHE:HD1	1:A:94:ILE:HD12	1.68	0.47
1:A:228:TYR:O	1:A:229:VAL:C	2.53	0.47
1:B:78:TRP:C	1:B:80:ILE:H	2.17	0.47
1:B:136:SER:O	1:B:137:ASN:HB3	2.13	0.47
1:A:329:LEU:O	1:A:330:LEU:C	2.53	0.47
1:A:362:MET:O	1:A:363:ILE:C	2.49	0.47
1:A:407:SER:OG	1:A:410:ARG:HB2	2.14	0.47
1:B:236:TYR:O	1:B:239:PHE:HB3	2.15	0.47
1:B:295:ALA:O	1:B:298:ILE:HB	2.15	0.47
1:B:311:SER:O	1:B:314:GLU:HB3	2.14	0.47
1:A:124:ALA:O	1:A:127:ALA:HB3	2.14	0.47
1:B:405:PRO:O	1:B:407:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:ND2	1:A:189:THR:OG1	2.48	0.47
1:A:391:GLY:O	1:A:395:ILE:HG13	2.14	0.47
1:B:1:MET:HA	1:B:5:LYS:HE3	1.97	0.47
1:B:38:ASN:HA	1:B:100:GLN:NE2	2.30	0.47
1:B:52:ILE:HG12	1:B:112:ILE:HG23	1.95	0.47
1:B:114:LEU:HD23	1:B:114:LEU:O	2.15	0.47
1:B:178:LEU:HG	1:B:179:ILE:N	2.30	0.47
1:B:210:LEU:O	1:B:213:ALA:HB3	2.13	0.47
1:B:245:ASN:O	1:B:248:THR:HB	2.15	0.47
1:B:271:LEU:HG	1:B:275:ILE:HD11	1.96	0.47
1:B:299:MET:O	1:B:300:SER:C	2.53	0.47
1:A:16:PHE:HE1	1:A:129:ILE:CG2	2.24	0.47
1:B:25:ALA:O	1:B:29:PHE:CB	2.62	0.47
1:B:70:LEU:HD11	1:B:76:LEU:HB2	1.96	0.47
1:B:91:PHE:HB3	1:B:170:PHE:CE2	2.49	0.47
1:B:93:PHE:CD1	1:B:93:PHE:N	2.82	0.47
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.50	0.47
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.97	0.47
1:A:212:LEU:HD22	1:A:345:PHE:CE1	2.49	0.47
1:A:223:TRP:HA	1:A:223:TRP:CE3	2.50	0.47
1:A:303:ILE:O	1:A:306:SER:N	2.39	0.47
1:A:400:LEU:HG	1:A:401:SER:N	2.30	0.47
1:A:379:GLN:O	1:A:382:TYR:HB2	2.15	0.47
1:B:45:THR:OG1	1:B:46:GLY:N	2.47	0.47
1:B:332:GLY:O	1:B:333:CYS:C	2.53	0.47
1:A:20:PHE:HD2	1:A:151:TRP:CB	2.16	0.46
1:A:235:THR:HG21	1:A:389:ALA:HB2	1.97	0.46
1:B:223:TRP:HA	1:B:223:TRP:HE3	1.81	0.46
1:A:37:ILE:CD1	1:A:162:PHE:CZ	2.95	0.46
1:A:260:VAL:O	1:A:261:PHE:C	2.50	0.46
1:B:18:PHE:CZ	1:B:180:LEU:CD1	2.98	0.46
1:B:85:VAL:HG22	1:B:178:LEU:CB	2.43	0.46
1:A:123:PRO:O	1:A:127:ALA:HB2	2.15	0.46
1:A:315:VAL:O	1:A:318:LEU:N	2.47	0.46
1:A:394:LEU:O	1:A:397:VAL:HB	2.15	0.46
1:B:154:GLY:O	1:B:155:ALA:C	2.54	0.46
1:B:247:PHE:HD2	1:B:315:VAL:CG1	2.27	0.46
1:A:9:PHE:HE2	1:A:10:TRP:CZ3	2.34	0.46
1:A:90:PHE:CZ	1:A:95:PHE:HE1	2.34	0.46
1:A:345:PHE:O	1:A:346:SER:C	2.54	0.46
1:B:239:PHE:CD1	1:B:240:ASP:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:SER:O	1:A:111:GLY:CA	2.64	0.46
1:A:193:SER:O	1:A:194:SER:CB	2.64	0.46
1:A:296:GLY:HA2	1:A:299:MET:CE	2.44	0.46
1:B:78:TRP:CD1	1:B:185:PHE:CE1	3.03	0.46
1:B:90:PHE:CZ	1:B:95:PHE:HE1	2.33	0.46
1:B:175:GLY:O	1:B:176:CYS:C	2.54	0.46
1:A:57:LEU:HD13	1:A:355:CYS:O	2.16	0.46
1:B:32:ILE:HD13	1:B:258:THR:HG23	1.97	0.46
1:B:100:GLN:C	1:B:102:ASN:H	2.17	0.46
1:B:320:THR:C	1:B:322:HIS:N	2.69	0.46
1:A:40:ILE:HG12	1:A:41:SER:O	2.16	0.46
1:A:157:ILE:CG2	1:A:161:MET:HG3	2.45	0.46
1:A:223:TRP:HA	1:A:223:TRP:HE3	1.81	0.46
1:B:85:VAL:O	1:B:174:SER:OG	2.34	0.46
1:B:234:CYS:SG	1:B:361:ALA:HB1	2.56	0.46
1:B:253:THR:CG2	1:B:254:GLY:N	2.79	0.46
1:B:382:TYR:N	1:B:382:TYR:CD1	2.83	0.46
1:A:236:TYR:CG	1:A:299:MET:SD	3.09	0.46
1:B:268:GLY:O	1:B:271:LEU:N	2.41	0.46
1:B:315:VAL:O	1:B:316:VAL:C	2.53	0.46
1:A:17:PHE:CD2	1:A:18:PHE:CE2	3.03	0.46
1:A:139:GLU:C	1:A:141:GLY:N	2.69	0.46
1:B:20:PHE:HB3	1:B:151:TRP:CB	2.46	0.46
1:B:89:PRO:O	1:B:93:PHE:HB2	2.16	0.46
1:A:20:PHE:CE2	1:A:148:CYS:HA	2.51	0.46
1:A:271:LEU:O	1:A:275:ILE:HG13	2.16	0.46
1:B:122:ALA:CB	1:B:123:PRO:CD	2.92	0.46
1:A:51:ALA:O	1:A:52:ILE:C	2.55	0.45
1:A:135:ARG:HH21	1:A:192:PRO:CA	2.29	0.45
1:B:27:PHE:HB3	1:B:28:PRO:HD3	1.94	0.45
1:B:107:SER:O	1:B:111:GLY:HA3	2.16	0.45
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.32	0.45
1:B:402:GLY:HA2	1:B:403:PRO:HD3	1.81	0.45
1:A:299:MET:O	1:A:300:SER:C	2.55	0.45
1:A:376:ILE:HG22	1:A:380:GLY:HA3	1.98	0.45
1:B:369:ALA:O	1:B:372:MET:HB2	2.16	0.45
1:A:113:TYR:O	1:A:116:PHE:CD2	2.70	0.45
1:B:63:PHE:CD1	1:B:63:PHE:C	2.90	0.45
1:A:120:ALA:O	1:A:123:PRO:HG2	2.16	0.45
1:A:30:PHE:O	1:A:31:PRO:C	2.51	0.45
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:CE2	1:B:148:CYS:HA	2.51	0.45
1:B:72:LEU:HG	1:B:72:LEU:O	2.17	0.45
1:B:224:PHE:N	1:B:224:PHE:HD1	2.13	0.45
1:B:228:TYR:OH	1:B:292:LEU:O	2.33	0.45
1:B:259:ARG:O	1:B:262:GLY:N	2.50	0.45
1:A:20:PHE:HB3	1:A:151:TRP:CB	2.46	0.45
1:A:26:TYR:HD1	1:A:27:PHE:N	2.13	0.45
1:A:208:PHE:CD2	1:A:351:LEU:HD13	2.52	0.45
1:B:23:MET:O	1:B:24:GLY:C	2.54	0.45
1:B:279:ALA:HB3	1:B:280:PRO:CD	2.38	0.45
1:B:362:MET:O	1:B:363:ILE:C	2.52	0.45
1:A:12:PHE:C	1:A:14:LEU:N	2.69	0.45
1:A:42:LYS:O	1:A:43:SER:C	2.55	0.45
1:A:116:PHE:C	1:A:116:PHE:CD1	2.88	0.45
1:A:175:GLY:O	1:A:176:CYS:C	2.55	0.45
1:B:12:PHE:C	1:B:14:LEU:N	2.70	0.45
1:B:193:SER:O	1:B:194:SER:CB	2.65	0.45
1:B:213:ALA:O	1:B:216:LEU:N	2.50	0.45
1:B:288:GLY:O	1:B:290:ASN:N	2.50	0.45
1:B:366:SER:O	1:B:369:ALA:HB3	2.17	0.45
1:B:370:GLY:HA2	1:B:373:TYR:HD2	1.82	0.45
1:A:11:MET:HA	1:A:11:MET:HE2	1.99	0.45
1:B:30:PHE:O	1:B:31:PRO:C	2.55	0.45
1:A:42:LYS:CE	1:A:373:TYR:HB3	2.47	0.44
1:A:75:TYR:CE2	1:A:79:ILE:HD11	2.52	0.44
1:A:104:LEU:O	1:A:108:ILE:HG13	2.17	0.44
1:A:325:GLU:O	1:A:326:VAL:C	2.55	0.44
1:B:33:TRP:HH2	1:B:95:PHE:CB	2.30	0.44
1:B:327:PRO:HG2	1:B:328:PHE:H	1.82	0.44
1:A:48:ILE:HG12	1:A:108:ILE:HG12	1.98	0.44
1:A:210:LEU:O	1:A:213:ALA:HB3	2.17	0.44
1:B:42:LYS:HB2	1:B:374:GLU:HB2	1.99	0.44
1:B:116:PHE:C	1:B:118:PHE:N	2.71	0.44
1:B:233:SER:O	1:B:234:CYS:C	2.56	0.44
1:B:236:TYR:OH	1:B:302:ARG:NH1	2.51	0.44
1:B:263:TYR:HD1	1:B:263:TYR:N	2.15	0.44
1:B:121:GLY:O	1:B:125:VAL:N	2.49	0.44
1:A:196:THR:HG21	1:A:201:VAL:CG1	2.48	0.44
1:B:38:ASN:CA	1:B:100:GLN:NE2	2.81	0.44
1:B:74:LYS:N	1:B:74:LYS:CD	2.72	0.44
1:B:85:VAL:CG1	1:B:178:LEU:HD22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:O	1:B:127:ALA:HB2	2.17	0.44
1:B:228:TYR:O	1:B:229:VAL:C	2.55	0.44
1:B:244:ALA:O	1:B:247:PHE:N	2.51	0.44
1:A:246:PHE:CD1	1:A:247:PHE:N	2.83	0.44
1:B:97:PRO:O	1:B:98:LEU:C	2.52	0.44
1:B:217:PHE:HD2	1:B:223:TRP:HH2	1.65	0.44
1:B:307:SER:O	1:B:379:GLN:NE2	2.50	0.44
1:B:345:PHE:O	1:B:346:SER:C	2.55	0.44
1:A:307:SER:HA	1:A:379:GLN:HB3	1.99	0.44
1:B:40:ILE:CG1	1:B:44:ASP:HB2	2.48	0.44
1:B:51:ALA:HB3	1:B:112:ILE:HD11	1.99	0.44
1:B:337:ILE:O	1:B:341:PHE:HB2	2.17	0.44
1:A:4:LEU:CD2	1:A:10:TRP:HZ3	2.28	0.44
1:A:89:PRO:O	1:A:93:PHE:HB2	2.17	0.44
1:B:38:ASN:CB	1:B:100:GLN:NE2	2.81	0.44
1:B:51:ALA:O	1:B:52:ILE:C	2.55	0.44
1:B:104:LEU:HG	1:B:108:ILE:HD11	1.99	0.44
1:B:336:TYR:CE2	1:B:400:LEU:HD11	2.52	0.44
1:A:250:PHE:CD1	1:A:250:PHE:N	2.86	0.44
1:B:329:LEU:HD12	1:B:329:LEU:HA	1.69	0.44
1:A:40:ILE:CG1	1:A:44:ASP:HB2	2.47	0.43
1:B:12:PHE:CE2	1:B:132:VAL:HG21	2.50	0.43
1:A:177:ALA:O	1:A:181:ALA:CB	2.65	0.43
1:A:264:VAL:O	1:A:267:MET:N	2.51	0.43
1:A:288:GLY:O	1:A:290:ASN:N	2.51	0.43
1:A:382:TYR:N	1:A:382:TYR:CD1	2.86	0.43
1:B:40:ILE:CD1	1:B:48:ILE:HD12	2.47	0.43
1:B:139:GLU:C	1:B:141:GLY:N	2.71	0.43
1:A:85:VAL:CG1	1:A:178:LEU:HD22	2.48	0.43
1:A:113:TYR:C	1:A:115:GLY:H	2.20	0.43
1:A:299:MET:O	1:A:302:ARG:N	2.51	0.43
1:A:340:GLN:C	1:A:341:PHE:CD1	2.91	0.43
1:B:307:SER:HA	1:B:379:GLN:HB3	2.00	0.43
1:B:260:VAL:O	1:B:261:PHE:C	2.55	0.43
1:B:391:GLY:O	1:B:395:ILE:HG13	2.18	0.43
1:A:40:ILE:CD1	1:A:48:ILE:HD12	2.49	0.43
1:A:135:ARG:NH2	1:A:192:PRO:C	2.72	0.43
1:B:13:GLY:O	1:B:146:PHE:CD2	2.70	0.43
1:B:134:ARG:NH1	1:B:203:ALA:CA	2.80	0.43
1:B:173:GLY:O	1:B:177:ALA:HB2	2.18	0.43
1:B:195:ALA:O	1:B:196:THR:CG2	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:CE1	1:A:113:TYR:CE1	3.07	0.43
1:A:188:LYS:HB2	1:A:189:THR:H	1.71	0.43
1:A:295:ALA:O	1:A:298:ILE:HB	2.19	0.43
1:B:50:ALA:O	1:B:51:ALA:C	2.57	0.43
1:B:124:ALA:O	1:B:127:ALA:HB3	2.19	0.43
1:B:373:TYR:HE1	1:B:382:TYR:CE1	2.36	0.43
1:A:53:SER:O	1:A:56:SER:N	2.48	0.43
1:B:57:LEU:HD13	1:B:355:CYS:O	2.19	0.43
1:B:320:THR:C	1:B:322:HIS:H	2.22	0.43
1:A:9:PHE:CD2	1:A:10:TRP:N	2.87	0.43
1:A:122:ALA:C	1:A:124:ALA:N	2.71	0.43
1:A:253:THR:CG2	1:A:254:GLY:N	2.81	0.43
1:B:11:MET:O	1:B:14:LEU:HB2	2.19	0.43
1:B:78:TRP:NE1	1:B:185:PHE:CD1	2.87	0.43
1:B:299:MET:O	1:B:302:ARG:N	2.52	0.43
1:A:18:PHE:CZ	1:A:180:LEU:HD12	2.53	0.43
1:A:96:GLY:O	1:A:100:GLN:N	2.40	0.43
1:B:23:MET:O	1:B:26:TYR:HB3	2.19	0.43
1:B:78:TRP:O	1:B:80:ILE:N	2.51	0.43
1:B:100:GLN:C	1:B:102:ASN:N	2.72	0.43
1:B:346:SER:O	1:B:347:ALA:C	2.57	0.43
1:A:26:TYR:O	1:A:27:PHE:C	2.58	0.43
1:A:227:LEU:O	1:A:228:TYR:C	2.56	0.43
1:A:233:SER:O	1:A:234:CYS:C	2.56	0.43
1:A:325:GLU:O	1:A:326:VAL:O	2.37	0.43
1:A:378:PHE:O	1:A:382:TYR:CD1	2.72	0.43
1:B:90:PHE:CD2	1:B:114:LEU:HD13	2.53	0.43
1:A:11:MET:O	1:A:14:LEU:HB2	2.19	0.42
1:A:346:SER:O	1:A:347:ALA:C	2.57	0.42
1:A:2:TYR:CE2	1:A:3:TYR:CD2	3.07	0.42
1:A:51:ALA:HB3	1:A:112:ILE:HD11	2.00	0.42
1:A:277:PHE:HD2	1:A:278:PHE:HE1	1.67	0.42
1:B:9:PHE:HE2	1:B:10:TRP:CZ3	2.36	0.42
1:B:319:LYS:O	1:B:321:LEU:N	2.52	0.42
1:B:326:VAL:HB	1:B:327:PRO:HD3	1.93	0.42
1:B:372:MET:O	1:B:376:ILE:HB	2.19	0.42
1:A:158:VAL:O	1:A:159:GLY:C	2.57	0.42
1:A:211:LYS:O	1:A:212:LEU:C	2.57	0.42
1:A:246:PHE:HB2	1:A:378:PHE:HD2	1.76	0.42
1:A:264:VAL:CG1	1:A:319:LYS:HG2	2.33	0.42
1:A:288:GLY:O	1:A:291:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:C	1:A:322:HIS:N	2.73	0.42
1:A:370:GLY:HA2	1:A:373:TYR:HD2	1.84	0.42
1:B:244:ALA:O	1:B:247:PHE:HB3	2.19	0.42
1:A:37:ILE:CD1	1:A:162:PHE:HZ	2.32	0.42
1:A:85:VAL:O	1:A:174:SER:OG	2.36	0.42
1:A:91:PHE:CD2	1:A:170:PHE:CZ	3.07	0.42
1:A:154:GLY:O	1:A:157:ILE:N	2.52	0.42
1:A:372:MET:O	1:A:376:ILE:HB	2.20	0.42
1:B:2:TYR:CE2	1:B:3:TYR:CD2	3.07	0.42
1:B:369:ALA:O	1:B:370:GLY:C	2.57	0.42
1:A:25:ALA:O	1:A:29:PHE:CB	2.67	0.42
1:A:42:LYS:HB2	1:A:374:GLU:HB2	2.00	0.42
1:A:53:SER:OG	1:A:363:ILE:HG13	2.20	0.42
1:A:78:TRP:CD1	1:A:185:PHE:CE1	3.08	0.42
1:B:113:TYR:O	1:B:116:PHE:CD2	2.70	0.42
1:B:177:ALA:O	1:B:181:ALA:CB	2.68	0.42
1:B:217:PHE:HD2	1:B:223:TRP:CH2	2.37	0.42
1:B:293:LEU:HD22	1:B:397:VAL:CG2	2.50	0.42
1:B:299:MET:O	1:B:303:ILE:HG13	2.20	0.42
1:A:42:LYS:HG3	1:A:374:GLU:CA	2.49	0.42
1:A:86:MET:C	1:A:89:PRO:HD2	2.40	0.42
1:A:125:VAL:O	1:A:129:ILE:HG13	2.20	0.42
1:A:312:ALA:O	1:A:315:VAL:HG23	2.18	0.42
1:B:20:PHE:O	1:B:24:GLY:N	2.47	0.42
1:B:296:GLY:HA2	1:B:299:MET:HE3	2.01	0.42
1:B:323:MET:HA	1:B:326:VAL:CG2	2.49	0.42
1:B:381:ALA:O	1:B:384:VAL:N	2.53	0.42
1:A:260:VAL:O	1:A:264:VAL:HG23	2.19	0.42
1:B:9:PHE:O	1:B:10:TRP:C	2.58	0.42
1:B:54:LEU:HA	1:B:363:ILE:HD11	2.01	0.42
1:B:373:TYR:O	1:B:377:GLY:N	2.44	0.42
1:A:263:TYR:O	1:A:264:VAL:C	2.58	0.42
1:A:279:ALA:HB3	1:A:280:PRO:CD	2.41	0.42
1:B:8:ASN:O	1:B:9:PHE:C	2.55	0.42
1:B:26:TYR:O	1:B:27:PHE:C	2.58	0.42
1:B:99:LEU:O	1:B:102:ASN:N	2.48	0.42
1:A:2:TYR:CE2	1:A:3:TYR:HD2	2.37	0.42
1:B:20:PHE:HD2	1:B:151:TRP:CB	2.18	0.42
1:B:22:ILE:H	1:B:22:ILE:HG13	1.64	0.42
1:B:40:ILE:HD11	1:B:45:THR:N	2.35	0.42
1:B:373:TYR:CE1	1:B:382:TYR:HE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HG	1:A:72:LEU:O	2.20	0.42
1:A:195:ALA:O	1:A:196:THR:CG2	2.63	0.42
1:A:273:ALA:O	1:A:274:SER:C	2.58	0.42
1:A:312:ALA:O	1:A:315:VAL:N	2.53	0.42
1:B:108:ILE:O	1:B:112:ILE:HG13	2.20	0.42
1:B:168:PHE:O	1:B:171:TRP:N	2.53	0.42
1:B:250:PHE:CD1	1:B:250:PHE:N	2.88	0.42
1:B:367:VAL:O	1:B:368:LEU:C	2.57	0.42
1:A:52:ILE:CA	1:A:112:ILE:HD13	2.50	0.41
1:B:60:GLN:O	1:B:60:GLN:HG2	2.19	0.41
1:B:264:VAL:CG1	1:B:319:LYS:HG2	2.37	0.41
1:A:8:ASN:O	1:A:9:PHE:C	2.56	0.41
1:A:10:TRP:HB3	1:A:11:MET:CE	2.49	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.87	0.41
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.50	0.41
1:A:299:MET:SD	1:A:325:GLU:OE2	2.78	0.41
1:A:327:PRO:HG2	1:A:328:PHE:H	1.84	0.41
1:B:42:LYS:O	1:B:43:SER:C	2.57	0.41
1:B:85:VAL:HG21	1:B:178:LEU:CD1	2.43	0.41
1:B:135:ARG:HH21	1:B:192:PRO:CA	2.33	0.41
1:A:90:PHE:CD2	1:A:114:LEU:HD13	2.50	0.41
1:B:351:LEU:HG	1:B:351:LEU:H	1.70	0.41
1:A:148:CYS:O	1:A:148:CYS:SG	2.76	0.41
1:A:268:GLY:O	1:A:271:LEU:N	2.39	0.41
1:B:107:SER:O	1:B:111:GLY:CA	2.68	0.41
1:A:10:TRP:NE1	1:B:168:PHE:CD1	2.85	0.41
1:A:116:PHE:C	1:A:118:PHE:N	2.73	0.41
1:A:193:SER:O	1:A:194:SER:HB3	2.21	0.41
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.68	0.41
1:B:33:TRP:CE3	1:B:38:ASN:ND2	2.89	0.41
1:B:158:VAL:O	1:B:159:GLY:C	2.58	0.41
1:B:271:LEU:O	1:B:275:ILE:HG13	2.20	0.41
1:B:372:MET:O	1:B:376:ILE:N	2.53	0.41
1:B:404:GLY:O	1:B:405:PRO:O	2.38	0.41
1:A:14:LEU:O	1:A:17:PHE:HB3	2.20	0.41
1:A:51:ALA:O	1:A:54:LEU:N	2.54	0.41
1:A:178:LEU:O	1:A:179:ILE:C	2.59	0.41
1:B:137:ASN:OD1	1:B:137:ASN:O	2.38	0.41
1:A:33:TRP:HH2	1:A:95:PHE:CB	2.34	0.41
1:A:40:ILE:HD11	1:A:45:THR:N	2.36	0.41
1:A:62:LEU:HD12	1:A:62:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:O	1:A:341:PHE:HB2	2.21	0.41
1:B:62:LEU:HD12	1:B:62:LEU:C	2.41	0.41
1:B:359:GLN:OE1	1:B:359:GLN:HA	2.19	0.41
1:B:370:GLY:O	1:B:371:ASN:C	2.58	0.41
1:A:85:VAL:CG1	1:A:178:LEU:HB2	2.49	0.41
1:A:208:PHE:CE2	1:A:351:LEU:HD13	2.56	0.41
1:A:250:PHE:O	1:A:312:ALA:HB2	2.21	0.41
1:B:157:ILE:HG23	1:B:161:MET:HG3	2.01	0.41
1:A:14:LEU:O	1:A:15:PHE:C	2.60	0.41
1:A:22:ILE:H	1:A:22:ILE:HG13	1.59	0.41
1:A:38:ASN:HA	1:A:100:GLN:NE2	2.36	0.41
1:A:86:MET:O	1:A:90:PHE:CB	2.69	0.41
1:A:192:PRO:HG2	1:A:197:VAL:HA	2.02	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.89	0.41
1:A:248:THR:HG22	1:A:248:THR:O	2.21	0.41
1:A:250:PHE:HD2	1:A:311:SER:C	2.23	0.41
1:A:277:PHE:HB3	1:A:278:PHE:CD1	2.55	0.41
1:B:40:ILE:HG13	1:B:44:ASP:CB	2.51	0.41
1:B:55:PHE:CZ	1:B:113:TYR:CE1	3.08	0.41
1:B:75:TYR:CE2	1:B:79:ILE:HD11	2.56	0.41
1:B:128:PHE:CE1	1:B:132:VAL:HG21	2.56	0.41
1:B:371:ASN:O	1:B:372:MET:C	2.59	0.41
1:B:381:ALA:O	1:B:382:TYR:C	2.60	0.41
1:A:38:ASN:HB3	1:A:100:GLN:NE2	2.36	0.41
1:A:44:ASP:HB3	1:A:104:LEU:CD1	2.51	0.41
1:A:52:ILE:HA	1:A:112:ILE:HD13	2.03	0.41
1:B:15:PHE:HD1	1:B:184:LEU:HD12	1.84	0.41
1:B:211:LYS:O	1:B:212:LEU:C	2.60	0.41
1:B:306:SER:O	1:B:379:GLN:NE2	2.54	0.41
1:A:31:PRO:O	1:A:34:LEU:HB2	2.22	0.40
1:A:367:VAL:O	1:A:368:LEU:C	2.60	0.40
1:A:381:ALA:O	1:A:382:TYR:C	2.59	0.40
1:B:55:PHE:HE1	1:B:113:TYR:HH	1.66	0.40
1:B:188:LYS:HB2	1:B:189:THR:H	1.71	0.40
1:B:264:VAL:O	1:B:267:MET:N	2.54	0.40
1:A:20:PHE:CD1	1:A:20:PHE:N	2.85	0.40
1:A:50:ALA:O	1:A:51:ALA:C	2.58	0.40
1:A:236:TYR:OH	1:A:302:ARG:NH1	2.54	0.40
1:A:303:ILE:C	1:A:305:GLY:N	2.70	0.40
1:B:63:PHE:CZ	1:B:124:ALA:HB2	2.55	0.40
1:B:288:GLY:O	1:B:291:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:O	1:A:24:GLY:N	2.49	0.40
1:A:302:ARG:O	1:A:302:ARG:HG2	2.20	0.40
1:A:337:ILE:O	1:A:338:THR:C	2.59	0.40
1:B:25:ALA:O	1:B:29:PHE:HB3	2.21	0.40
1:B:90:PHE:CE2	1:B:95:PHE:CE1	3.04	0.40
1:B:276:MET:C	1:B:278:PHE:N	2.75	0.40
1:A:216:LEU:CD2	1:A:219:GLN:OE1	2.66	0.40
1:A:275:ILE:CG2	1:A:327:PRO:HG3	2.43	0.40
1:A:386:GLY:O	1:A:389:ALA:HB3	2.21	0.40
1:A:387:LEU:O	1:A:388:VAL:C	2.58	0.40
1:B:23:MET:O	1:B:24:GLY:O	2.39	0.40
1:B:289:LYS:CG	1:B:400:LEU:HD23	2.24	0.40
1:A:10:TRP:CZ2	1:B:168:PHE:CD1	3.10	0.40
1:A:179:ILE:O	1:A:183:LEU:HB2	2.22	0.40
1:A:247:PHE:HD2	1:A:315:VAL:CG1	2.34	0.40
1:A:372:MET:O	1:A:376:ILE:N	2.54	0.40
1:B:34:LEU:HD22	1:B:40:ILE:HD12	2.04	0.40
1:B:273:ALA:O	1:B:274:SER:C	2.59	0.40
1:B:314:GLU:O	1:B:318:LEU:HG	2.22	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	415/417 (100%)	274 (66%)	102 (25%)	39 (9%)	0	8
1	B	415/417 (100%)	271 (65%)	107 (26%)	37 (9%)	1	8
All	All	830/834 (100%)	545 (66%)	209 (25%)	76 (9%)	1	8

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	26	TYR
1	A	117	CYS
1	A	196	THR
1	A	264	VAL
1	A	320	THR
1	A	326	VAL
1	A	346	SER
1	A	406	LEU
1	B	2	TYR
1	B	26	TYR
1	B	108	ILE
1	B	117	CYS
1	B	160	ILE
1	B	264	VAL
1	B	320	THR
1	B	326	VAL
1	B	406	LEU
1	A	39	HIS
1	A	108	ILE
1	A	137	ASN
1	A	160	ILE
1	A	165	ASN
1	A	228	TYR
1	A	402	GLY
1	A	407	SER
1	B	137	ASN
1	B	165	ASN
1	B	196	THR
1	B	321	LEU
1	B	346	SER
1	B	402	GLY
1	B	405	PRO
1	B	407	SER
1	A	35	HIS
1	A	102	ASN
1	A	321	LEU
1	A	343	VAL
1	A	405	PRO
1	B	24	GLY
1	B	35	HIS
1	B	102	ASN
1	B	228	TYR

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Mol	Chain	Res	Type
1	B	343	VAL
1	A	11	MET
1	A	30	PHE
1	A	194	SER
1	B	30	PHE
1	B	75	TYR
1	B	103	ILE
1	B	124	ALA
1	B	250	PHE
1	A	24	GLY
1	A	75	TYR
1	A	103	ILE
1	B	96	GLY
1	B	289	LYS
1	B	378	PHE
1	A	239	PHE
1	A	378	PHE
1	B	27	PHE
1	A	27	PHE
1	A	229	VAL
1	B	327	PRO
1	A	96	GLY
1	A	179	ILE
1	A	327	PRO
1	B	229	VAL
1	B	112	ILE
1	B	238	VAL
1	A	112	ILE
1	A	238	VAL
1	A	370	GLY
1	B	28	PRO
1	B	109	VAL
1	A	79	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	345/345 (100%)	317 (92%)	28 (8%)	11 41
1	B	345/345 (100%)	317 (92%)	28 (8%)	11 41
All	All	690/690 (100%)	634 (92%)	56 (8%)	11 41

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	10	TRP
1	A	30	PHE
1	A	53	SER
1	A	59	PHE
1	A	62	LEU
1	A	91	PHE
1	A	107	SER
1	A	116	PHE
1	A	135	ARG
1	A	136	SER
1	A	138	PHE
1	A	163	THR
1	A	171	TRP
1	A	239	PHE
1	A	241	GLN
1	A	246	PHE
1	A	278	PHE
1	A	280	PRO
1	A	315	VAL
1	A	323	MET
1	A	324	PHE
1	A	325	GLU
1	A	333	CYS
1	A	355	CYS
1	A	379	GLN
1	A	398	PHE
1	A	401	SER
1	B	3	TYR
1	B	10	TRP
1	B	30	PHE
1	B	53	SER
1	B	59	PHE
1	B	62	LEU
1	B	91	PHE

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Mol	Chain	Res	Type
1	B	107	SER
1	B	116	PHE
1	B	135	ARG
1	B	136	SER
1	B	138	PHE
1	B	171	TRP
1	B	239	PHE
1	B	241	GLN
1	B	246	PHE
1	B	249	SER
1	B	278	PHE
1	B	280	PRO
1	B	315	VAL
1	B	323	MET
1	B	324	PHE
1	B	325	GLU
1	B	333	CYS
1	B	355	CYS
1	B	379	GLN
1	B	398	PHE
1	B	401	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	ASN
1	A	60	GLN
1	A	100	GLN
1	A	102	ASN
1	A	119	ASN
1	A	137	ASN
1	A	204	ASN
1	A	241	GLN
1	A	242	GLN
1	A	290	ASN
1	A	340	GLN
1	A	379	GLN
1	B	8	ASN
1	B	38	ASN
1	B	60	GLN
1	B	100	GLN

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	119	ASN
1	B	137	ASN
1	B	204	ASN
1	B	241	GLN
1	B	242	GLN
1	B	290	ASN
1	B	340	GLN
1	B	379	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.