Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:54 AM GMT

PDB ID	:	2V8N
Title	:	WILD-TYPE STRUCTURE OF LACTOSE PERMEASE
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Deposited on	:	2007-08-09
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

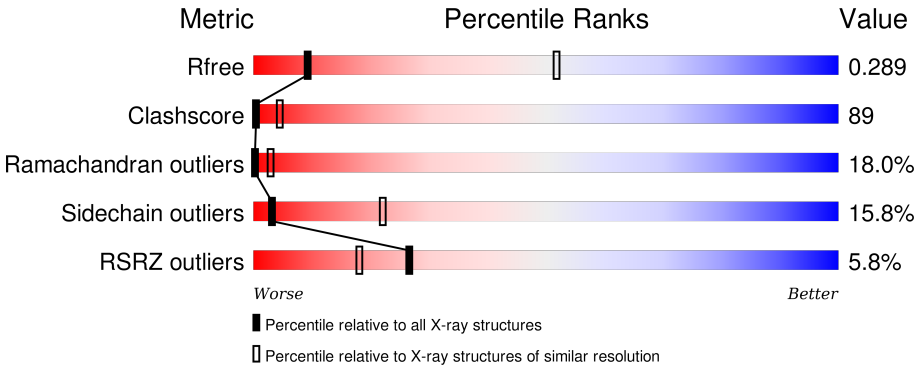
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	417	5% 20% 55% 24%
1	B	417	6% 19% 56% 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6584 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.

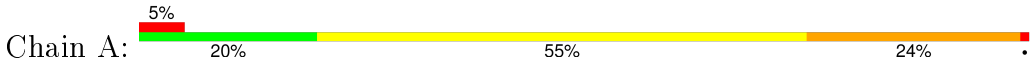
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3292	2223	506	541	22			
1	B	417	Total	C	N	O	S	0	0	0
			3292	2223	506	541	22			

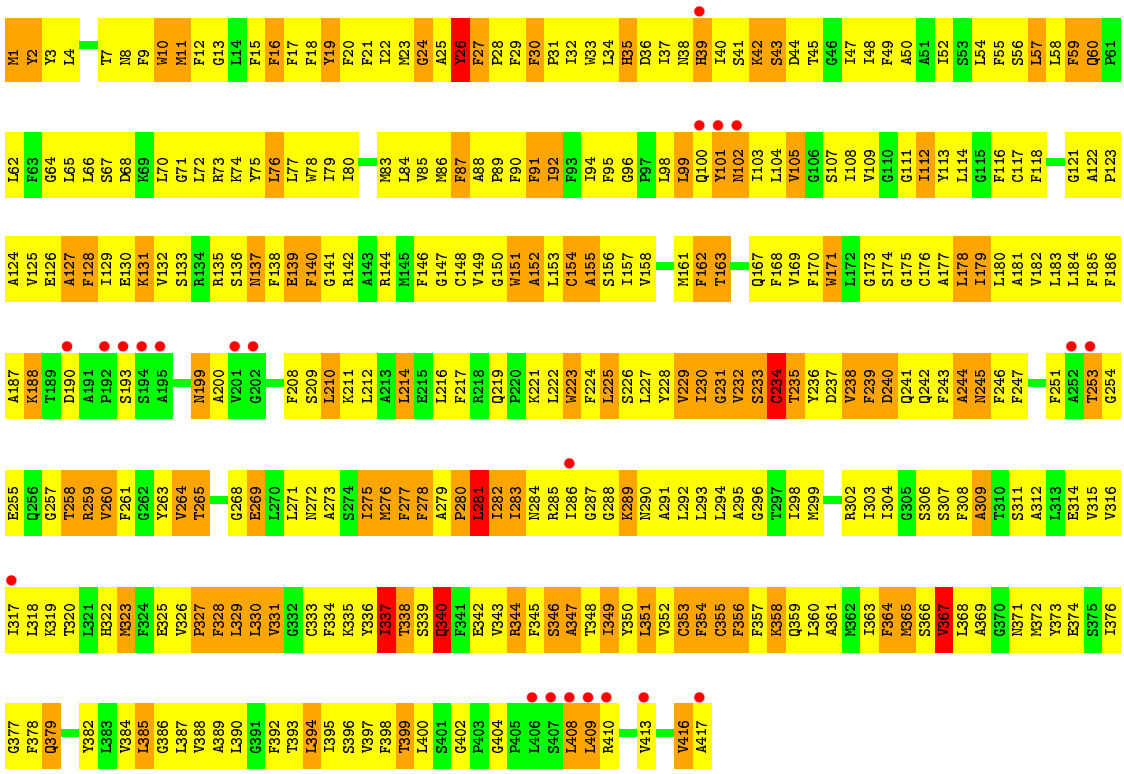
3 Residue-property plots (i)

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

- Molecule 1: LACTOSE PERMEASE

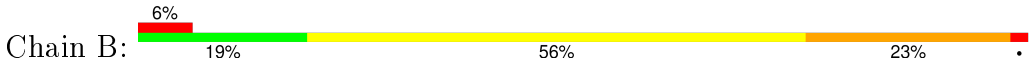
Chain A:

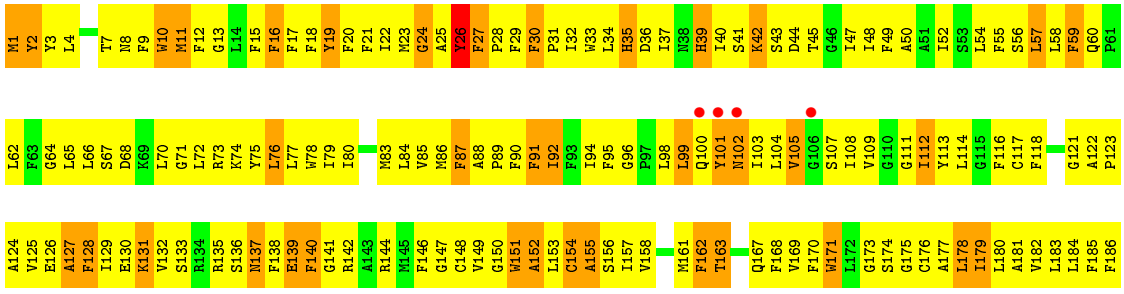


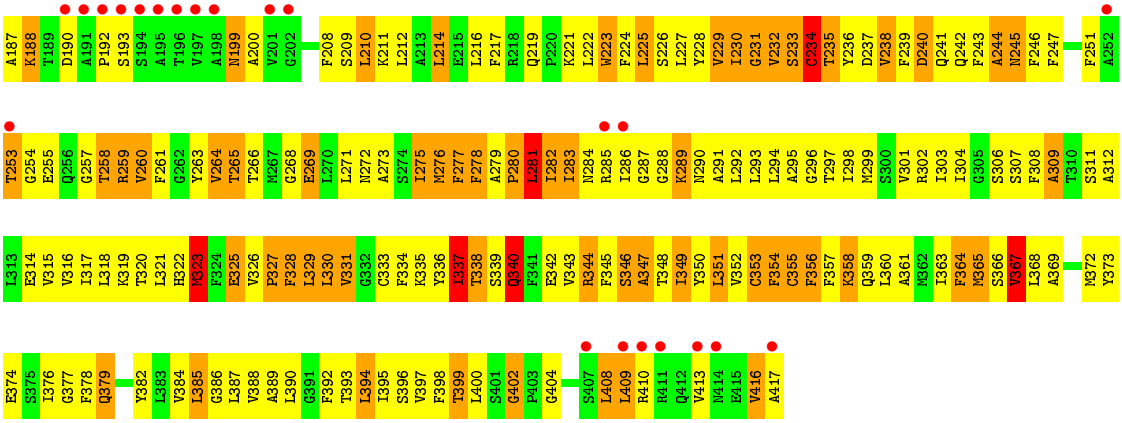


- Molecule 1: LACTOSE PERMEASE

Chain B:






A187 K188 T189 D190 A191 P192 S193 S194 A195 T196 V197 A198 N199 A200 V201 G202 F208 S209 L210 K211 L212 A213 L214 E215 L216 F217 R218 Q219 P220 K221 L222 W223 F224 L225 S226 L227 Y228 V229 I230 G231 V232 S233 C234 T235 Y236 D237 V238 F239 D240 Q241 Q242 F243 A244 N245 F246 F247 F251 A252
T253 G254 E255 Q256 G257 T258 R259 V260 F261 G262 Y263 V264 T265 T266 W267 G268 E269 L270 L271 N272 A273 S274 I275 M276 F277 F278 A279 P280 L281 I282 I283 N284 R285 I286 G287 G288 K289 N290 A291 L292 L293 L294 A295 G296 T297 I298 M299 S300 V301 R302 I303 I304 G305 S306 S307 F308 A309 T310 S311 A312
L313 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 V352 C353 F354 C355 F356 F357 K358 Q359 L360 A361 M362 I363 F364 M365 S366 V367 L368 A369 M372 Y373
E374 S375 I376 G377 F378 Q379 Y382 L383 V384 L385 G386 L387 V388 A389 L390 G391 F392 T393 L394 I395 S396 V397 F398 T399 L400 S401 G402 P403 G404 S407 L408 L409 R410 R411 Q412 V413 W414 E415 V416 A417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.37Å 127.40Å 188.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.60 34.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	82.7 (10.00-3.60) 84.3 (34.51-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.47Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.294 , 0.333 0.308 , 0.289	Depositor DCC
R_{free} test set	1177 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	87.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.18$	Xtriage
Outliers	4 of 26405 reflections (0.015%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	6584	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.59	0/3389	0.79	1/4591 (0.0%)
1	B	0.60	1/3389 (0.0%)	0.79	1/4591 (0.0%)
All	All	0.60	1/6778 (0.0%)	0.79	2/9182 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	CYS	CB-SG	5.31	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	234	CYS	CA-CB-SG	7.08	126.75	114.00
1	A	234	CYS	CA-CB-SG	6.98	126.57	114.00

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	3292	0	3335	584	0
1	B	3292	0	3335	595	0
All	All	6584	0	6670	1178	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 89.

All (1178) 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:264:VAL:HG13	1:B:265:THR:H	1.09	1.10
1:B:302:ARG:HH22	1:B:319:LYS:HD2	1.10	1.09
1:B:396:SER:HA	1:B:399:THR:HB	1.33	1.09
1:A:396:SER:HA	1:A:399:THR:HB	1.34	1.09
1:A:302:ARG:HH22	1:A:319:LYS:HD2	1.09	1.08
1:A:264:VAL:HG13	1:A:265:THR:H	1.11	1.07
1:A:246:PHE:HB2	1:A:378:PHE:CD2	1.91	1.06
1:B:246:PHE:HB2	1:B:378:PHE:CD2	1.90	1.05
1:A:246:PHE:HB2	1:A:378:PHE:HD2	1.18	1.05
1:A:22:ILE:HD11	1:A:177:ALA:HB2	1.42	1.02
1:B:22:ILE:HD11	1:B:177:ALA:HB2	1.42	1.02
1:B:385:LEU:HA	1:B:388:VAL:HG12	1.40	0.99
1:B:246:PHE:HB2	1:B:378:PHE:HD2	1.17	0.99
1:A:385:LEU:HA	1:A:388:VAL:HG12	1.42	0.99
1:A:139:GLU:HG2	1:A:141:GLY:H	1.26	0.99
1:B:30:PHE:HB3	1:B:31:PRO:HD3	1.44	0.98
1:A:281:LEU:HD22	1:A:281:LEU:H	1.23	0.98
1:B:139:GLU:HG2	1:B:141:GLY:H	1.27	0.97
1:B:281:LEU:HD22	1:B:281:LEU:H	1.24	0.97
1:A:30:PHE:HB3	1:A:31:PRO:HD3	1.46	0.94
1:B:272:ASN:HB2	1:B:323:MET:HG3	1.50	0.94
1:A:272:ASN:HB2	1:A:323:MET:HG3	1.50	0.94
1:B:413:VAL:HG13	1:B:417:ALA:HB3	1.49	0.94
1:B:210:LEU:HD23	1:B:210:LEU:H	1.30	0.93
1:A:413:VAL:HG13	1:A:417:ALA:HB3	1.50	0.93
1:A:210:LEU:HD23	1:A:210:LEU:H	1.32	0.93
1:B:209:SER:HB3	1:B:212:LEU:HB2	1.51	0.93
1:A:302:ARG:NH2	1:A:319:LYS:HD2	1.84	0.93
1:B:238:VAL:O	1:B:241:GLN:HG2	1.69	0.92
1:B:302:ARG:NH2	1:B:319:LYS:HD2	1.84	0.92
1:B:289:LYS:HE3	1:B:400:LEU:HB3	1.52	0.91
1:A:230:ILE:O	1:A:234:CYS:HB3	1.70	0.91
1:A:33:TRP:HA	1:A:37:ILE:HD12	1.53	0.91
1:B:311:SER:HB2	1:B:314:GLU:HB2	1.53	0.91
1:A:209:SER:HB3	1:A:212:LEU:HB2	1.52	0.90
1:A:311:SER:HB2	1:A:314:GLU:HB2	1.54	0.89
1:B:264:VAL:HG13	1:B:265:THR:N	1.87	0.89
1:B:33:TRP:HA	1:B:37:ILE:HD12	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:HA	1:A:261:PHE:CZ	2.08	0.89
1:B:26:TYR:O	1:B:30:PHE:HB2	1.73	0.88
1:B:45:THR:HG22	1:B:48:ILE:HD12	1.56	0.88
1:B:302:ARG:HH21	1:B:322:HIS:HB2	1.39	0.88
1:A:26:TYR:O	1:A:30:PHE:HB2	1.72	0.88
1:B:230:ILE:O	1:B:234:CYS:HB3	1.73	0.87
1:A:289:LYS:HE3	1:A:400:LEU:HB3	1.54	0.87
1:A:238:VAL:O	1:A:241:GLN:HG2	1.75	0.87
1:B:29:PHE:HA	1:B:261:PHE:CZ	2.10	0.86
1:A:264:VAL:HG13	1:A:265:THR:N	1.89	0.86
1:B:19:TYR:O	1:B:22:ILE:HG22	1.76	0.86
1:A:73:ARG:C	1:A:74:LYS:HD2	1.96	0.86
1:B:73:ARG:C	1:B:74:LYS:HD2	1.96	0.86
1:A:302:ARG:HH21	1:A:322:HIS:HB2	1.41	0.85
1:A:19:TYR:O	1:A:22:ILE:HG22	1.76	0.85
1:A:45:THR:HG22	1:A:48:ILE:HD12	1.56	0.85
1:A:211:LYS:HA	1:A:214:LEU:HD22	1.58	0.84
1:A:392:PHE:HA	1:A:395:ILE:HG22	1.59	0.83
1:A:29:PHE:HA	1:A:261:PHE:HZ	1.40	0.83
1:B:261:PHE:O	1:B:264:VAL:HG12	1.79	0.82
1:B:272:ASN:OD1	1:B:275:ILE:HD11	1.79	0.82
1:A:355:CYS:C	1:A:357:PHE:H	1.82	0.82
1:B:302:ARG:NH2	1:B:319:LYS:HA	1.94	0.82
1:B:392:PHE:HA	1:B:395:ILE:HG22	1.59	0.82
1:A:251:PHE:HB2	1:A:257:GLY:HA2	1.61	0.82
1:B:355:CYS:C	1:B:357:PHE:H	1.83	0.82
1:B:385:LEU:HA	1:B:388:VAL:CG1	2.09	0.81
1:A:302:ARG:NH2	1:A:319:LYS:HA	1.94	0.81
1:B:211:LYS:HA	1:B:214:LEU:HD22	1.59	0.81
1:B:29:PHE:HA	1:B:261:PHE:HZ	1.43	0.81
1:A:258:THR:O	1:A:260:VAL:N	2.13	0.81
1:A:7:THR:HG23	1:A:8:ASN:H	1.45	0.81
1:B:104:LEU:O	1:B:108:ILE:HG12	1.81	0.80
1:A:177:ALA:O	1:A:181:ALA:HB3	1.81	0.80
1:B:177:ALA:O	1:B:181:ALA:HB3	1.80	0.80
1:A:24:GLY:HA2	1:A:151:TRP:CZ3	2.17	0.80
1:A:385:LEU:HA	1:A:388:VAL:CG1	2.11	0.80
1:B:251:PHE:HB2	1:B:257:GLY:HA2	1.62	0.80
1:A:104:LEU:O	1:A:108:ILE:HG12	1.82	0.80
1:B:174:SER:O	1:B:177:ALA:HB3	1.82	0.80
1:A:264:VAL:HG21	1:A:319:LYS:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ASN:OD1	1:A:275:ILE:HD11	1.81	0.79
1:B:258:THR:O	1:B:260:VAL:N	2.15	0.79
1:B:264:VAL:HG21	1:B:319:LYS:HG2	1.65	0.79
1:B:7:THR:HG23	1:B:8:ASN:H	1.46	0.79
1:A:233:SER:O	1:A:236:TYR:HB3	1.82	0.78
1:A:55:PHE:O	1:A:59:PHE:HB2	1.83	0.78
1:B:233:SER:O	1:B:236:TYR:HB3	1.83	0.78
1:B:55:PHE:O	1:B:59:PHE:HB2	1.83	0.78
1:A:261:PHE:O	1:A:264:VAL:HG12	1.84	0.78
1:B:24:GLY:HA2	1:B:151:TRP:CZ3	2.19	0.78
1:B:42:LYS:HD3	1:B:42:LYS:H	1.48	0.77
1:B:243:PHE:O	1:B:246:PHE:HB3	1.85	0.77
1:B:279:ALA:O	1:B:283:ILE:HG12	1.85	0.77
1:A:330:LEU:HD12	1:A:331:VAL:HG12	1.67	0.76
1:A:281:LEU:N	1:A:281:LEU:HD22	1.98	0.76
1:B:282:ILE:O	1:B:286:ILE:HG12	1.85	0.76
1:A:243:PHE:O	1:A:246:PHE:HB3	1.85	0.76
1:B:210:LEU:O	1:B:214:LEU:HD13	1.85	0.76
1:A:174:SER:O	1:A:177:ALA:HB3	1.86	0.76
1:A:234:CYS:HB2	1:A:358:LYS:HE2	1.66	0.76
1:B:281:LEU:HD22	1:B:281:LEU:N	1.99	0.76
1:A:279:ALA:O	1:A:283:ILE:HG12	1.85	0.76
1:A:112:ILE:C	1:A:114:LEU:H	1.89	0.76
1:A:282:ILE:O	1:A:286:ILE:HG12	1.86	0.75
1:A:76:LEU:HD12	1:A:79:ILE:HD12	1.69	0.75
1:B:16:PHE:HD2	1:B:144:ARG:HA	1.52	0.75
1:B:112:ILE:C	1:B:114:LEU:H	1.88	0.75
1:A:355:CYS:O	1:A:357:PHE:N	2.19	0.75
1:A:16:PHE:HD2	1:A:144:ARG:HA	1.50	0.75
1:B:234:CYS:HB2	1:B:358:LYS:HE2	1.68	0.74
1:B:76:LEU:HD12	1:B:79:ILE:HD12	1.68	0.74
1:A:234:CYS:HB2	1:A:358:LYS:CE	2.16	0.74
1:A:279:ALA:HB3	1:A:280:PRO:HD3	1.69	0.74
1:B:35:HIS:O	1:B:39:HIS:HA	1.87	0.74
1:B:234:CYS:HB2	1:B:358:LYS:CE	2.17	0.74
1:B:88:ALA:HB3	1:B:89:PRO:HD3	1.69	0.74
1:A:62:LEU:H	1:A:62:LEU:HD12	1.52	0.74
1:B:62:LEU:HD12	1:B:62:LEU:H	1.53	0.74
1:A:221:LYS:HD3	1:A:340:GLN:HG3	1.69	0.74
1:A:22:ILE:CD1	1:A:177:ALA:HB2	2.18	0.73
1:B:330:LEU:HD12	1:B:331:VAL:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:HIS:O	1:A:39:HIS:HA	1.89	0.73
1:A:48:ILE:O	1:A:52:ILE:HG13	1.89	0.73
1:B:355:CYS:O	1:B:357:PHE:N	2.20	0.73
1:B:279:ALA:HB3	1:B:280:PRO:HD3	1.68	0.73
1:B:48:ILE:O	1:B:52:ILE:HG13	1.87	0.73
1:B:15:PHE:HD1	1:B:184:LEU:HD12	1.52	0.73
1:B:302:ARG:HH22	1:B:319:LYS:HA	1.52	0.73
1:B:52:ILE:HG12	1:B:112:ILE:HG21	1.70	0.72
1:B:308:PHE:O	1:B:309:ALA:C	2.27	0.72
1:A:52:ILE:HG12	1:A:112:ILE:HG21	1.69	0.72
1:A:80:ILE:O	1:A:84:LEU:HD23	1.90	0.72
1:B:337:ILE:O	1:B:338:THR:C	2.27	0.72
1:A:337:ILE:O	1:A:338:THR:C	2.28	0.72
1:A:349:ILE:H	1:A:349:ILE:HD12	1.54	0.72
1:B:22:ILE:CD1	1:B:177:ALA:HB2	2.18	0.72
1:A:210:LEU:O	1:A:214:LEU:HD13	1.90	0.72
1:A:302:ARG:HH22	1:A:319:LYS:HA	1.52	0.72
1:B:349:ILE:HD12	1:B:349:ILE:H	1.55	0.72
1:A:15:PHE:HD1	1:A:184:LEU:HD12	1.54	0.72
1:A:227:LEU:HA	1:A:230:ILE:HD12	1.72	0.72
1:B:22:ILE:CG2	1:B:23:MET:N	2.53	0.72
1:B:157:ILE:HD11	1:B:168:PHE:HE2	1.55	0.72
1:B:259:ARG:C	1:B:261:PHE:H	1.92	0.71
1:A:88:ALA:HB2	1:A:170:PHE:C	2.11	0.71
1:A:157:ILE:HD11	1:A:168:PHE:HE2	1.53	0.71
1:A:259:ARG:C	1:A:261:PHE:H	1.92	0.71
1:B:258:THR:O	1:B:261:PHE:N	2.23	0.71
1:B:368:LEU:O	1:B:372:MET:HB2	1.90	0.71
1:B:88:ALA:HB2	1:B:170:PHE:C	2.11	0.71
1:A:42:LYS:H	1:A:42:LYS:HD3	1.53	0.71
1:A:258:THR:O	1:A:261:PHE:N	2.22	0.70
1:A:312:ALA:O	1:A:316:VAL:HG23	1.91	0.70
1:A:22:ILE:CG2	1:A:23:MET:N	2.54	0.70
1:B:244:ALA:O	1:B:246:PHE:N	2.25	0.70
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.72	0.70
1:A:308:PHE:O	1:A:309:ALA:C	2.27	0.70
1:B:231:GLY:HA3	1:B:392:PHE:CD2	2.27	0.70
1:B:312:ALA:O	1:B:316:VAL:HG23	1.91	0.70
1:A:128:PHE:CD1	1:A:129:ILE:HD13	2.27	0.69
1:A:244:ALA:O	1:A:246:PHE:N	2.25	0.69
1:B:227:LEU:HA	1:B:230:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:CE2	1:A:95:PHE:HB2	2.26	0.69
1:B:90:PHE:CE2	1:B:95:PHE:HB2	2.27	0.69
1:B:268:GLY:O	1:B:272:ASN:N	2.25	0.69
1:B:76:LEU:CD1	1:B:79:ILE:HD12	2.23	0.69
1:B:41:SER:HB3	1:B:44:ASP:OD2	1.92	0.69
1:B:379:GLN:H	1:B:379:GLN:HE21	1.41	0.69
1:B:80:ILE:O	1:B:84:LEU:HD23	1.93	0.69
1:B:278:PHE:C	1:B:281:LEU:HD23	2.13	0.69
1:B:221:LYS:HD3	1:B:340:GLN:HG3	1.73	0.69
1:B:40:ILE:HG13	1:B:44:ASP:HB2	1.75	0.69
1:A:273:ALA:O	1:A:276:MET:HB3	1.92	0.69
1:A:40:ILE:HG13	1:A:44:ASP:HB2	1.75	0.69
1:A:128:PHE:C	1:A:128:PHE:CD1	2.66	0.68
1:A:21:PHE:CD1	1:A:154:CYS:HB2	2.28	0.68
1:A:157:ILE:HD11	1:A:168:PHE:CE2	2.27	0.68
1:B:296:GLY:HA2	1:B:299:MET:HE3	1.75	0.68
1:A:76:LEU:CD1	1:A:79:ILE:HD12	2.22	0.68
1:A:41:SER:HB3	1:A:44:ASP:OD2	1.94	0.68
1:B:128:PHE:CD1	1:B:129:ILE:HD13	2.28	0.68
1:B:273:ALA:O	1:B:276:MET:HB3	1.94	0.68
1:A:368:LEU:O	1:A:372:MET:HB2	1.92	0.68
1:A:176:CYS:O	1:A:180:LEU:HB2	1.93	0.68
1:A:44:ASP:O	1:A:47:ILE:HG22	1.94	0.68
1:A:231:GLY:HA3	1:A:392:PHE:CD2	2.28	0.68
1:B:281:LEU:O	1:B:285:ARG:HB2	1.94	0.68
1:B:128:PHE:CD1	1:B:128:PHE:C	2.66	0.68
1:A:302:ARG:NH2	1:A:319:LYS:O	2.27	0.68
1:A:128:PHE:HD1	1:A:129:ILE:N	1.92	0.68
1:A:278:PHE:C	1:A:281:LEU:HD23	2.15	0.68
1:B:111:GLY:C	1:B:113:TYR:H	1.95	0.68
1:A:285:ARG:O	1:A:286:ILE:HD13	1.95	0.67
1:B:302:ARG:NH2	1:B:319:LYS:O	2.27	0.67
1:B:176:CYS:O	1:B:180:LEU:HB2	1.93	0.67
1:B:44:ASP:O	1:B:47:ILE:HG22	1.94	0.67
1:B:211:LYS:CA	1:B:214:LEU:HD22	2.24	0.67
1:A:225:LEU:HD23	1:A:226:SER:N	2.09	0.67
1:B:157:ILE:HD11	1:B:168:PHE:CE2	2.29	0.67
1:A:255:GLU:O	1:A:259:ARG:HB2	1.94	0.67
1:A:268:GLY:O	1:A:272:ASN:N	2.25	0.67
1:A:382:TYR:O	1:A:386:GLY:N	2.25	0.67
1:B:255:GLU:O	1:B:259:ARG:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:H	1:A:408:LEU:HD23	1.60	0.67
1:A:169:VAL:HG23	1:A:170:PHE:N	2.10	0.67
1:B:128:PHE:HD1	1:B:129:ILE:N	1.93	0.67
1:A:283:ILE:O	1:A:287:GLY:N	2.28	0.67
1:B:21:PHE:CD1	1:B:154:CYS:HB2	2.28	0.67
1:B:76:LEU:O	1:B:79:ILE:N	2.27	0.67
1:A:258:THR:OG1	1:A:259:ARG:N	2.29	0.67
1:B:22:ILE:HG22	1:B:23:MET:N	2.09	0.67
1:B:225:LEU:HD23	1:B:226:SER:N	2.10	0.66
1:A:320:THR:C	1:A:322:HIS:H	1.99	0.66
1:A:319:LYS:O	1:A:322:HIS:HB2	1.95	0.66
1:A:379:GLN:HE21	1:A:379:GLN:H	1.42	0.66
1:B:319:LYS:O	1:B:322:HIS:HB2	1.94	0.66
1:B:279:ALA:C	1:B:283:ILE:HG12	2.16	0.66
1:B:112:ILE:H	1:B:112:ILE:CD1	2.08	0.66
1:A:22:ILE:HG22	1:A:23:MET:N	2.10	0.66
1:A:76:LEU:O	1:A:79:ILE:N	2.28	0.66
1:A:111:GLY:C	1:A:113:TYR:H	1.96	0.66
1:A:279:ALA:C	1:A:283:ILE:HG12	2.16	0.66
1:B:385:LEU:CA	1:B:388:VAL:HG12	2.19	0.66
1:B:283:ILE:O	1:B:287:GLY:N	2.29	0.66
1:B:285:ARG:O	1:B:286:ILE:HD13	1.96	0.66
1:B:162:PHE:CG	1:B:163:THR:N	2.63	0.65
1:A:112:ILE:CD1	1:A:112:ILE:H	2.09	0.65
1:A:162:PHE:CG	1:A:163:THR:N	2.64	0.65
1:B:254:GLY:O	1:B:258:THR:HG23	1.96	0.65
1:A:169:VAL:HG23	1:A:170:PHE:H	1.62	0.65
1:A:20:PHE:O	1:A:24:GLY:N	2.29	0.65
1:A:72:LEU:HD11	1:A:131:LYS:HD3	1.79	0.65
1:B:48:ILE:HG22	1:B:52:ILE:HD11	1.77	0.65
1:A:281:LEU:O	1:A:285:ARG:HB2	1.96	0.65
1:B:258:THR:OG1	1:B:259:ARG:N	2.30	0.65
1:A:251:PHE:HB2	1:A:257:GLY:CA	2.26	0.65
1:B:408:LEU:HD23	1:B:408:LEU:H	1.62	0.65
1:A:169:VAL:HG23	1:A:170:PHE:HD1	1.62	0.65
1:A:211:LYS:CA	1:A:214:LEU:HD22	2.24	0.65
1:A:355:CYS:C	1:A:357:PHE:N	2.51	0.64
1:A:48:ILE:HG22	1:A:52:ILE:HD11	1.79	0.64
1:A:312:ALA:O	1:A:315:VAL:HG22	1.98	0.64
1:B:199:ASN:HD22	1:B:200:ALA:N	1.96	0.64
1:A:29:PHE:CA	1:A:261:PHE:HZ	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HD13	1:A:331:VAL:N	2.12	0.64
1:B:169:VAL:HG23	1:B:170:PHE:N	2.12	0.64
1:B:251:PHE:HB2	1:B:257:GLY:CA	2.27	0.64
1:B:72:LEU:HD11	1:B:131:LYS:HD3	1.79	0.64
1:B:337:ILE:O	1:B:340:GLN:N	2.31	0.64
1:A:337:ILE:O	1:A:340:GLN:N	2.31	0.64
1:A:359:GLN:O	1:A:363:ILE:HG13	1.98	0.64
1:B:320:THR:C	1:B:322:HIS:H	2.00	0.64
1:A:345:PHE:HB3	1:A:349:ILE:HD11	1.80	0.64
1:B:29:PHE:CA	1:B:261:PHE:HZ	2.11	0.64
1:B:345:PHE:HB3	1:B:349:ILE:HD11	1.80	0.64
1:B:234:CYS:H	1:B:358:LYS:HZ1	1.44	0.64
1:A:302:ARG:O	1:A:306:SER:OG	2.16	0.63
1:B:20:PHE:O	1:B:24:GLY:N	2.30	0.63
1:B:154:CYS:O	1:B:157:ILE:HG22	1.98	0.63
1:B:312:ALA:O	1:B:315:VAL:HG22	1.99	0.63
1:A:337:ILE:CD1	1:A:350:TYR:HE1	2.11	0.63
1:A:385:LEU:CA	1:A:388:VAL:HG12	2.21	0.63
1:B:330:LEU:HD13	1:B:331:VAL:N	2.13	0.63
1:A:154:CYS:O	1:A:157:ILE:HG22	1.99	0.63
1:A:229:VAL:HG12	1:A:358:LYS:HE3	1.81	0.63
1:B:355:CYS:C	1:B:357:PHE:N	2.52	0.63
1:B:122:ALA:N	1:B:123:PRO:HD2	2.12	0.63
1:B:169:VAL:HG23	1:B:170:PHE:HD1	1.63	0.63
1:B:52:ILE:HG23	1:B:112:ILE:HG21	1.81	0.63
1:A:112:ILE:C	1:A:114:LEU:N	2.51	0.63
1:A:45:THR:HA	1:A:48:ILE:HD12	1.79	0.63
1:B:337:ILE:CD1	1:B:350:TYR:HE1	2.11	0.63
1:B:104:LEU:H	1:B:104:LEU:HD12	1.63	0.63
1:B:216:LEU:HD12	1:B:219:GLN:NE2	2.14	0.63
1:B:42:LYS:H	1:B:42:LYS:CD	2.08	0.63
1:A:254:GLY:O	1:A:258:THR:HG23	1.98	0.63
1:A:122:ALA:N	1:A:123:PRO:HD2	2.12	0.63
1:B:112:ILE:HD13	1:B:112:ILE:N	2.13	0.63
1:A:155:ALA:O	1:A:158:VAL:HG22	1.99	0.63
1:A:112:ILE:N	1:A:112:ILE:HD13	2.14	0.62
1:B:139:GLU:HG2	1:B:141:GLY:N	2.09	0.62
1:A:7:THR:HG23	1:A:8:ASN:N	2.14	0.62
1:B:289:LYS:HG2	1:B:400:LEU:HD23	1.82	0.62
1:B:45:THR:HA	1:B:48:ILE:HD12	1.81	0.62
1:A:104:LEU:H	1:A:104:LEU:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:HD22	1:A:200:ALA:N	1.96	0.62
1:B:230:ILE:O	1:B:231:GLY:C	2.37	0.62
1:B:7:THR:HG23	1:B:8:ASN:N	2.14	0.62
1:B:112:ILE:C	1:B:114:LEU:N	2.49	0.62
1:B:26:TYR:CD1	1:B:27:PHE:N	2.67	0.62
1:A:216:LEU:HD12	1:A:219:GLN:NE2	2.14	0.62
1:A:33:TRP:CE3	1:A:34:LEU:HD23	2.35	0.62
1:A:136:SER:O	1:A:137:ASN:HB2	1.99	0.62
1:A:337:ILE:HD13	1:A:350:TYR:HE1	1.65	0.62
1:A:35:HIS:O	1:A:39:HIS:N	2.32	0.62
1:A:121:GLY:O	1:A:124:ALA:HB3	2.00	0.62
1:B:351:LEU:C	1:B:351:LEU:CD2	2.69	0.62
1:B:234:CYS:SG	1:B:365:MET:HG3	2.40	0.61
1:A:275:ILE:CD1	1:A:327:PRO:HB3	2.30	0.61
1:A:33:TRP:CA	1:A:37:ILE:HD12	2.28	0.61
1:A:52:ILE:HG23	1:A:112:ILE:HG21	1.82	0.61
1:B:392:PHE:CA	1:B:395:ILE:HG22	2.29	0.61
1:A:275:ILE:HD13	1:A:327:PRO:HB3	1.83	0.61
1:B:337:ILE:HD13	1:B:350:TYR:HE1	1.65	0.61
1:B:179:ILE:O	1:B:183:LEU:HB2	2.01	0.61
1:A:139:GLU:HG2	1:A:141:GLY:N	2.08	0.61
1:B:128:PHE:CE1	1:B:129:ILE:HD13	2.36	0.61
1:B:16:PHE:CD2	1:B:144:ARG:HA	2.35	0.61
1:B:229:VAL:HG12	1:B:358:LYS:HE3	1.81	0.61
1:A:271:LEU:C	1:A:271:LEU:HD23	2.20	0.61
1:B:359:GLN:O	1:B:363:ILE:HG13	2.00	0.61
1:B:121:GLY:O	1:B:124:ALA:HB3	2.01	0.61
1:B:35:HIS:O	1:B:39:HIS:N	2.32	0.61
1:A:117:CYS:O	1:A:121:GLY:HA3	1.99	0.61
1:B:117:CYS:O	1:B:121:GLY:HA3	2.01	0.61
1:B:136:SER:O	1:B:137:ASN:HB2	2.00	0.61
1:A:16:PHE:CD2	1:A:144:ARG:HA	2.33	0.61
1:B:155:ALA:O	1:B:158:VAL:HG22	2.01	0.61
1:B:167:GLN:O	1:B:171:TRP:HB2	2.00	0.61
1:B:30:PHE:HB3	1:B:31:PRO:CD	2.26	0.61
1:A:128:PHE:CD1	1:A:129:ILE:N	2.69	0.61
1:B:337:ILE:HG21	1:B:349:ILE:HG21	1.82	0.61
1:B:323:MET:HE3	1:B:326:VAL:HG21	1.83	0.61
1:B:275:ILE:CD1	1:B:327:PRO:HB3	2.30	0.61
1:A:272:ASN:O	1:A:275:ILE:HG13	2.01	0.61
1:A:44:ASP:O	1:A:48:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:CD1	1:B:129:ILE:N	2.69	0.61
1:B:140:PHE:HD1	1:B:140:PHE:H	1.49	0.61
1:B:169:VAL:HG23	1:B:170:PHE:H	1.63	0.60
1:B:271:LEU:C	1:B:271:LEU:HD23	2.21	0.60
1:A:296:GLY:HA2	1:A:299:MET:HE3	1.83	0.60
1:A:179:ILE:O	1:A:183:LEU:HB2	1.99	0.60
1:B:272:ASN:O	1:B:275:ILE:HG13	2.01	0.60
1:A:26:TYR:CD1	1:A:27:PHE:N	2.69	0.60
1:B:416:VAL:HG12	1:B:416:VAL:O	2.02	0.60
1:B:302:ARG:O	1:B:306:SER:OG	2.17	0.60
1:B:311:SER:O	1:B:315:VAL:HG13	2.01	0.60
1:A:392:PHE:CA	1:A:395:ILE:HG22	2.29	0.60
1:A:128:PHE:CE1	1:A:129:ILE:HD13	2.36	0.60
1:B:282:ILE:HG23	1:B:286:ILE:HG13	1.83	0.60
1:B:154:CYS:O	1:B:156:SER:N	2.34	0.60
1:B:244:ALA:O	1:B:247:PHE:N	2.34	0.60
1:B:33:TRP:CE3	1:B:34:LEU:HD23	2.37	0.60
1:A:49:PHE:CD2	1:A:241:GLN:HB2	2.36	0.60
1:A:52:ILE:HA	1:A:112:ILE:HG13	1.82	0.60
1:B:351:LEU:C	1:B:351:LEU:HD23	2.21	0.60
1:A:54:LEU:HD23	1:A:54:LEU:C	2.22	0.60
1:B:33:TRP:CA	1:B:37:ILE:HD12	2.29	0.60
1:A:289:LYS:HG2	1:A:400:LEU:HD23	1.83	0.60
1:A:244:ALA:O	1:A:247:PHE:N	2.34	0.60
1:B:99:LEU:HD23	1:B:107:SER:HB3	1.83	0.60
1:A:57:LEU:HD12	1:A:359:GLN:HB2	1.83	0.60
1:B:246:PHE:HZ	1:B:309:ALA:CB	2.15	0.60
1:A:167:GLN:O	1:A:171:TRP:HB2	2.00	0.60
1:B:231:GLY:O	1:B:235:THR:HG23	2.01	0.60
1:A:154:CYS:O	1:A:156:SER:N	2.35	0.60
1:A:9:PHE:HD2	1:A:10:TRP:HE3	1.48	0.60
1:B:303:ILE:HB	1:B:386:GLY:HA2	1.82	0.60
1:A:272:ASN:HB2	1:A:323:MET:CG	2.30	0.60
1:B:9:PHE:HD2	1:B:10:TRP:HE3	1.48	0.60
1:B:272:ASN:HB2	1:B:323:MET:CG	2.30	0.59
1:A:254:GLY:O	1:A:258:THR:N	2.34	0.59
1:A:351:LEU:C	1:A:351:LEU:CD2	2.70	0.59
1:B:241:GLN:HE22	1:B:366:SER:HB2	1.66	0.59
1:A:337:ILE:HG21	1:A:349:ILE:HG21	1.83	0.59
1:B:78:TRP:CZ2	1:B:185:PHE:HB3	2.38	0.59
1:A:140:PHE:H	1:A:140:PHE:HD1	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:HZ	1:A:309:ALA:CB	2.15	0.59
1:A:116:PHE:CG	1:A:117:CYS:N	2.71	0.59
1:A:416:VAL:O	1:A:416:VAL:HG12	2.02	0.59
1:B:2:TYR:H	1:B:2:TYR:HD1	1.49	0.59
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.38	0.59
1:B:413:VAL:HG13	1:B:417:ALA:CB	2.29	0.59
1:B:54:LEU:HD23	1:B:54:LEU:C	2.23	0.59
1:B:44:ASP:O	1:B:48:ILE:HG13	2.02	0.59
1:B:275:ILE:HD13	1:B:327:PRO:HB3	1.83	0.59
1:A:282:ILE:HG23	1:A:286:ILE:HG13	1.83	0.59
1:B:232:VAL:O	1:B:236:TYR:CB	2.50	0.59
1:B:246:PHE:HB2	1:B:378:PHE:CE2	2.37	0.59
1:A:232:VAL:CG1	1:A:299:MET:HE3	2.32	0.59
1:A:351:LEU:C	1:A:351:LEU:HD23	2.23	0.59
1:B:49:PHE:CD2	1:B:241:GLN:HB2	2.38	0.59
1:A:23:MET:O	1:A:25:ALA:N	2.36	0.59
1:A:251:PHE:CE2	1:A:260:VAL:HG21	2.38	0.58
1:B:90:PHE:O	1:B:94:ILE:N	2.26	0.58
1:A:232:VAL:O	1:A:236:TYR:CB	2.52	0.58
1:B:23:MET:O	1:B:25:ALA:N	2.36	0.58
1:B:227:LEU:CA	1:B:230:ILE:HD12	2.34	0.58
1:B:52:ILE:HA	1:B:112:ILE:HG13	1.85	0.58
1:A:112:ILE:HD13	1:A:112:ILE:H	1.67	0.58
1:A:331:VAL:HG23	1:A:335:LYS:HD3	1.84	0.58
1:A:234:CYS:H	1:A:358:LYS:HZ1	1.49	0.58
1:B:211:LYS:HA	1:B:214:LEU:CD2	2.31	0.58
1:B:104:LEU:H	1:B:104:LEU:CD1	2.16	0.58
1:A:330:LEU:CD1	1:A:331:VAL:N	2.66	0.58
1:B:382:TYR:O	1:B:386:GLY:N	2.24	0.58
1:A:241:GLN:HE22	1:A:366:SER:HB2	1.67	0.58
1:B:112:ILE:HD13	1:B:112:ILE:H	1.67	0.58
1:B:302:ARG:NH2	1:B:319:LYS:CA	2.66	0.58
1:A:211:LYS:HA	1:A:214:LEU:CD2	2.31	0.58
1:A:15:PHE:CD1	1:A:184:LEU:HD12	2.36	0.58
1:A:2:TYR:H	1:A:2:TYR:HD1	1.50	0.58
1:A:234:CYS:SG	1:A:365:MET:HG3	2.44	0.58
1:B:337:ILE:HD13	1:B:350:TYR:CE1	2.39	0.58
1:B:127:ALA:O	1:B:130:GLU:N	2.33	0.58
1:A:99:LEU:HD23	1:A:107:SER:HB3	1.85	0.58
1:B:282:ILE:C	1:B:286:ILE:HG12	2.24	0.58
1:A:78:TRP:CZ2	1:A:185:PHE:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:HB	1:A:386:GLY:HA2	1.85	0.58
1:B:331:VAL:HG23	1:B:335:LYS:HD3	1.85	0.58
1:A:231:GLY:HA3	1:A:392:PHE:CE2	2.38	0.57
1:B:54:LEU:O	1:B:54:LEU:HD23	2.04	0.57
1:B:231:GLY:HA3	1:B:392:PHE:CE2	2.39	0.57
1:B:392:PHE:HA	1:B:395:ILE:CG2	2.30	0.57
1:A:234:CYS:H	1:A:358:LYS:NZ	2.01	0.57
1:A:337:ILE:HD13	1:A:350:TYR:CE1	2.39	0.57
1:A:129:ILE:O	1:A:133:SER:HB3	2.04	0.57
1:B:234:CYS:H	1:B:358:LYS:NZ	2.02	0.57
1:A:295:ALA:HB2	1:A:328:PHE:HB3	1.85	0.57
1:B:224:PHE:HA	1:B:227:LEU:HD12	1.86	0.57
1:A:231:GLY:O	1:A:235:THR:HG23	2.05	0.57
1:A:413:VAL:HG13	1:A:417:ALA:CB	2.30	0.57
1:A:251:PHE:CZ	1:A:260:VAL:HG21	2.38	0.57
1:A:94:ILE:O	1:A:98:LEU:HD13	2.05	0.57
1:B:330:LEU:CD1	1:B:331:VAL:N	2.67	0.57
1:A:169:VAL:HG23	1:A:170:PHE:CD1	2.39	0.57
1:A:311:SER:O	1:A:315:VAL:HG13	2.04	0.57
1:B:35:HIS:O	1:B:39:HIS:CA	2.52	0.57
1:B:348:THR:O	1:B:352:VAL:N	2.37	0.57
1:A:224:PHE:HA	1:A:227:LEU:HD12	1.87	0.57
1:A:50:ALA:HB2	1:A:366:SER:OG	2.04	0.57
1:A:211:LYS:O	1:A:212:LEU:C	2.43	0.57
1:B:57:LEU:HD11	1:B:360:LEU:HB2	1.87	0.57
1:B:251:PHE:CE2	1:B:260:VAL:HG21	2.40	0.57
1:A:104:LEU:H	1:A:104:LEU:CD1	2.17	0.57
1:B:351:LEU:HD22	1:B:352:VAL:N	2.20	0.57
1:B:105:VAL:O	1:B:109:VAL:HG23	2.05	0.57
1:B:234:CYS:SG	1:B:361:ALA:HB1	2.44	0.57
1:B:23:MET:C	1:B:25:ALA:H	2.08	0.57
1:B:15:PHE:CD1	1:B:184:LEU:HD12	2.36	0.57
1:A:365:MET:O	1:A:368:LEU:HB2	2.05	0.56
1:A:90:PHE:O	1:A:94:ILE:N	2.28	0.56
1:B:232:VAL:CG1	1:B:299:MET:HE3	2.35	0.56
1:A:230:ILE:O	1:A:231:GLY:C	2.42	0.56
1:B:116:PHE:CG	1:B:117:CYS:N	2.73	0.56
1:B:251:PHE:CZ	1:B:260:VAL:HG21	2.40	0.56
1:B:261:PHE:O	1:B:264:VAL:CG1	2.51	0.56
1:B:275:ILE:HD13	1:B:327:PRO:HD3	1.88	0.56
1:B:238:VAL:HG13	1:B:366:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:THR:O	1:A:352:VAL:N	2.38	0.56
1:A:282:ILE:O	1:A:283:ILE:C	2.42	0.56
1:B:295:ALA:O	1:B:298:ILE:HB	2.05	0.56
1:A:234:CYS:SG	1:A:361:ALA:HB1	2.45	0.56
1:A:23:MET:C	1:A:25:ALA:H	2.08	0.56
1:B:57:LEU:HD12	1:B:359:GLN:HB2	1.87	0.56
1:B:259:ARG:C	1:B:261:PHE:N	2.59	0.56
1:A:351:LEU:HD22	1:A:352:VAL:N	2.21	0.56
1:A:127:ALA:O	1:A:130:GLU:N	2.34	0.56
1:A:282:ILE:C	1:A:286:ILE:HG12	2.26	0.56
1:A:30:PHE:HB3	1:A:31:PRO:CD	2.27	0.56
1:B:177:ALA:O	1:B:181:ALA:CB	2.53	0.56
1:B:129:ILE:O	1:B:133:SER:HB3	2.05	0.56
1:B:17:PHE:HA	1:B:147:GLY:HA2	1.88	0.56
1:B:229:VAL:O	1:B:233:SER:HB3	2.06	0.56
1:B:254:GLY:O	1:B:258:THR:N	2.35	0.56
1:B:365:MET:O	1:B:368:LEU:HB2	2.06	0.56
1:A:168:PHE:HE1	1:B:186:PHE:HB2	1.71	0.56
1:A:17:PHE:HA	1:A:147:GLY:HA2	1.87	0.56
1:A:35:HIS:O	1:A:39:HIS:CA	2.53	0.56
1:B:94:ILE:O	1:B:98:LEU:HD13	2.06	0.56
1:A:229:VAL:O	1:A:233:SER:HB3	2.05	0.56
1:A:105:VAL:O	1:A:109:VAL:HG23	2.06	0.56
1:A:392:PHE:HA	1:A:395:ILE:CG2	2.31	0.55
1:B:190:ASP:O	1:B:192:PRO:HD3	2.06	0.55
1:B:112:ILE:N	1:B:112:ILE:CD1	2.70	0.55
1:B:33:TRP:CH2	1:B:96:GLY:HA2	2.41	0.55
1:A:210:LEU:H	1:A:210:LEU:CD2	2.08	0.55
1:B:376:ILE:HG22	1:B:376:ILE:O	2.07	0.55
1:B:235:THR:HG22	1:B:365:MET:SD	2.46	0.55
1:A:259:ARG:C	1:A:261:PHE:N	2.59	0.55
1:A:277:PHE:O	1:A:280:PRO:HD2	2.05	0.55
1:A:227:LEU:CA	1:A:230:ILE:HD12	2.34	0.55
1:A:33:TRP:CH2	1:A:96:GLY:HA2	2.41	0.55
1:B:57:LEU:HD12	1:B:360:LEU:N	2.22	0.55
1:A:54:LEU:O	1:A:54:LEU:HD23	2.06	0.55
1:A:280:PRO:O	1:A:281:LEU:C	2.45	0.55
1:B:277:PHE:O	1:B:280:PRO:HD2	2.06	0.55
1:B:348:THR:O	1:B:352:VAL:HB	2.06	0.55
1:B:278:PHE:HA	1:B:281:LEU:CD2	2.36	0.55
1:B:150:GLY:O	1:B:154:CYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:O	1:B:92:ILE:HG22	2.06	0.55
1:A:376:ILE:HG22	1:A:376:ILE:O	2.07	0.55
1:A:349:ILE:N	1:A:349:ILE:HD12	2.21	0.55
1:B:357:PHE:O	1:B:360:LEU:HB3	2.07	0.55
1:B:55:PHE:CE2	1:B:113:TYR:HA	2.42	0.55
1:B:337:ILE:CG2	1:B:349:ILE:HG21	2.37	0.55
1:A:1:MET:O	1:A:4:LEU:HB2	2.07	0.54
1:A:299:MET:O	1:A:302:ARG:HB3	2.06	0.54
1:B:342:GLU:O	1:B:344:ARG:N	2.39	0.54
1:A:59:PHE:O	1:A:62:LEU:N	2.39	0.54
1:A:188:LYS:C	1:A:188:LYS:HD2	2.28	0.54
1:B:169:VAL:HG23	1:B:170:PHE:CD1	2.41	0.54
1:A:275:ILE:HD13	1:A:327:PRO:HD3	1.88	0.54
1:A:52:ILE:CG1	1:A:112:ILE:HG21	2.37	0.54
1:A:295:ALA:O	1:A:298:ILE:HB	2.06	0.54
1:A:302:ARG:NH2	1:A:319:LYS:CA	2.67	0.54
1:B:219:GLN:O	1:B:222:LEU:HB3	2.07	0.54
1:B:368:LEU:O	1:B:372:MET:N	2.35	0.54
1:A:342:GLU:O	1:A:344:ARG:N	2.40	0.54
1:A:42:LYS:CD	1:A:42:LYS:H	2.12	0.54
1:A:278:PHE:HA	1:A:281:LEU:CD2	2.38	0.54
1:A:135:ARG:HD2	1:A:135:ARG:C	2.28	0.54
1:B:188:LYS:HD2	1:B:188:LYS:C	2.28	0.54
1:B:28:PRO:HG2	1:B:29:PHE:H	1.72	0.54
1:B:295:ALA:HB2	1:B:328:PHE:HB3	1.88	0.54
1:A:357:PHE:O	1:A:360:LEU:HB3	2.06	0.54
1:B:67:SER:HA	1:B:71:GLY:O	2.06	0.54
1:B:389:ALA:O	1:B:392:PHE:HB2	2.08	0.54
1:A:219:GLN:O	1:A:222:LEU:HB3	2.08	0.54
1:A:251:PHE:CB	1:A:257:GLY:HA2	2.34	0.54
1:A:389:ALA:O	1:A:392:PHE:HB2	2.07	0.54
1:A:17:PHE:CE1	1:A:150:GLY:HA2	2.43	0.54
1:B:76:LEU:HD12	1:B:79:ILE:HB	1.90	0.54
1:B:306:SER:O	1:B:379:GLN:HG3	2.08	0.54
1:B:241:GLN:NE2	1:B:366:SER:HB2	2.23	0.54
1:A:76:LEU:HD12	1:A:79:ILE:HB	1.90	0.54
1:B:394:LEU:O	1:B:397:VAL:HG23	2.08	0.54
1:A:369:ALA:HA	1:A:372:MET:CB	2.38	0.54
1:A:238:VAL:HG13	1:A:366:SER:HA	1.90	0.53
1:A:348:THR:O	1:A:352:VAL:HB	2.07	0.53
1:B:282:ILE:O	1:B:283:ILE:C	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LYS:O	1:B:214:LEU:N	2.42	0.53
1:B:232:VAL:O	1:B:236:TYR:HB2	2.08	0.53
1:B:344:ARG:HG2	1:B:345:PHE:HD1	1.73	0.53
1:A:337:ILE:CG2	1:A:349:ILE:HG21	2.38	0.53
1:B:99:LEU:H	1:B:99:LEU:HD23	1.73	0.53
1:A:101:TYR:O	1:A:103:ILE:HG12	2.08	0.53
1:A:92:ILE:O	1:A:92:ILE:HG22	2.06	0.53
1:B:323:MET:CE	1:B:326:VAL:HG21	2.38	0.53
1:A:55:PHE:CE2	1:A:113:TYR:HA	2.44	0.53
1:B:59:PHE:O	1:B:62:LEU:N	2.41	0.53
1:B:237:ASP:O	1:B:240:ASP:N	2.41	0.53
1:B:88:ALA:HB2	1:B:170:PHE:O	2.09	0.53
1:A:258:THR:O	1:A:259:ARG:C	2.46	0.53
1:A:150:GLY:O	1:A:154:CYS:HB2	2.08	0.53
1:B:210:LEU:CD2	1:B:210:LEU:H	2.07	0.53
1:B:111:GLY:C	1:B:113:TYR:N	2.62	0.53
1:B:12:PHE:HE2	1:B:128:PHE:HE1	1.57	0.53
1:A:67:SER:HA	1:A:71:GLY:O	2.09	0.53
1:B:398:PHE:O	1:B:399:THR:C	2.47	0.53
1:A:296:GLY:HA2	1:A:299:MET:CE	2.38	0.53
1:A:33:TRP:HA	1:A:37:ILE:CD1	2.34	0.53
1:A:241:GLN:NE2	1:A:366:SER:HB2	2.24	0.53
1:A:368:LEU:O	1:A:372:MET:N	2.36	0.53
1:A:12:PHE:HE2	1:A:128:PHE:HE1	1.57	0.53
1:B:182:VAL:HA	1:B:185:PHE:HD2	1.74	0.53
1:B:101:TYR:O	1:B:103:ILE:N	2.42	0.53
1:B:390:LEU:O	1:B:394:LEU:HB3	2.09	0.53
1:A:232:VAL:O	1:A:236:TYR:HB2	2.08	0.53
1:B:85:VAL:O	1:B:174:SER:HB3	2.08	0.53
1:B:1:MET:O	1:B:4:LEU:HB2	2.08	0.53
1:B:384:VAL:O	1:B:388:VAL:HB	2.09	0.53
1:A:88:ALA:HB2	1:A:170:PHE:O	2.09	0.53
1:B:208:PHE:CE2	1:B:348:THR:HG22	2.43	0.53
1:B:379:GLN:H	1:B:379:GLN:NE2	2.06	0.53
1:A:211:LYS:O	1:A:214:LEU:N	2.41	0.53
1:B:333:CYS:O	1:B:334:PHE:C	2.47	0.53
1:B:336:TYR:OH	1:B:400:LEU:HD11	2.08	0.53
1:B:307:SER:O	1:B:379:GLN:HG2	2.09	0.53
1:B:369:ALA:HA	1:B:372:MET:CB	2.39	0.52
1:A:326:VAL:N	1:A:327:PRO:HD2	2.24	0.52
1:A:398:PHE:O	1:A:399:THR:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LYS:O	1:B:212:LEU:C	2.46	0.52
1:A:99:LEU:HD23	1:A:99:LEU:H	1.73	0.52
1:B:90:PHE:CZ	1:B:95:PHE:HB2	2.44	0.52
1:A:394:LEU:O	1:A:397:VAL:HG23	2.09	0.52
1:A:90:PHE:CZ	1:A:95:PHE:HB2	2.44	0.52
1:B:280:PRO:O	1:B:281:LEU:C	2.47	0.52
1:B:349:ILE:HD12	1:B:349:ILE:N	2.23	0.52
1:B:116:PHE:CD2	1:B:117:CYS:N	2.77	0.52
1:A:135:ARG:HD2	1:A:135:ARG:O	2.09	0.52
1:A:28:PRO:HG2	1:A:29:PHE:H	1.74	0.52
1:B:101:TYR:O	1:B:103:ILE:HG12	2.09	0.52
1:B:258:THR:O	1:B:259:ARG:C	2.47	0.52
1:B:52:ILE:HG23	1:B:112:ILE:CG2	2.39	0.52
1:A:52:ILE:HG23	1:A:112:ILE:CG2	2.39	0.52
1:A:272:ASN:HA	1:A:275:ILE:HG12	1.91	0.52
1:A:306:SER:O	1:A:379:GLN:HG3	2.09	0.52
1:B:17:PHE:CE1	1:B:150:GLY:HA2	2.44	0.52
1:B:135:ARG:HD2	1:B:135:ARG:C	2.29	0.52
1:A:390:LEU:O	1:A:394:LEU:HB3	2.09	0.52
1:B:22:ILE:HG22	1:B:23:MET:H	1.72	0.52
1:A:111:GLY:C	1:A:113:TYR:N	2.62	0.52
1:B:128:PHE:CZ	1:B:132:VAL:HG21	2.45	0.52
1:B:104:LEU:N	1:B:104:LEU:HD12	2.24	0.52
1:B:52:ILE:CG1	1:B:112:ILE:HG21	2.39	0.52
1:A:29:PHE:HE2	1:A:170:PHE:CE1	2.28	0.52
1:A:333:CYS:O	1:A:334:PHE:C	2.47	0.52
1:B:351:LEU:CD2	1:B:352:VAL:N	2.73	0.52
1:A:101:TYR:O	1:A:103:ILE:N	2.42	0.52
1:B:33:TRP:HA	1:B:37:ILE:CD1	2.35	0.52
1:B:369:ALA:O	1:B:373:TYR:CD2	2.62	0.52
1:A:369:ALA:HA	1:A:372:MET:HB3	1.92	0.52
1:A:16:PHE:CZ	1:A:126:GLU:HA	2.44	0.52
1:B:303:ILE:HG21	1:B:385:LEU:HD12	1.91	0.52
1:A:344:ARG:HG2	1:A:345:PHE:HD1	1.75	0.51
1:A:177:ALA:O	1:A:181:ALA:CB	2.54	0.51
1:A:59:PHE:HA	1:A:62:LEU:HD13	1.91	0.51
1:B:59:PHE:HA	1:B:62:LEU:HD13	1.91	0.51
1:B:29:PHE:HE2	1:B:170:PHE:CE1	2.28	0.51
1:B:272:ASN:HA	1:B:275:ILE:HG12	1.91	0.51
1:A:307:SER:O	1:A:379:GLN:HG2	2.10	0.51
1:A:323:MET:CE	1:A:326:VAL:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG22	1:A:23:MET:H	1.75	0.51
1:B:268:GLY:O	1:B:271:LEU:HB3	2.10	0.51
1:A:85:VAL:O	1:A:174:SER:HB3	2.10	0.51
1:B:135:ARG:O	1:B:135:ARG:HD2	2.11	0.51
1:B:388:VAL:CG1	1:B:389:ALA:N	2.74	0.51
1:A:226:SER:O	1:A:230:ILE:HG13	2.11	0.51
1:A:345:PHE:O	1:A:347:ALA:N	2.44	0.51
1:A:385:LEU:C	1:A:387:LEU:N	2.64	0.51
1:A:388:VAL:CG1	1:A:389:ALA:N	2.73	0.51
1:A:182:VAL:HA	1:A:185:PHE:HD2	1.74	0.51
1:B:251:PHE:CB	1:B:257:GLY:HA2	2.35	0.51
1:A:232:VAL:HG11	1:A:299:MET:HE3	1.93	0.51
1:A:268:GLY:O	1:A:271:LEU:HB3	2.10	0.51
1:A:116:PHE:CD2	1:A:117:CYS:N	2.76	0.51
1:B:55:PHE:HE2	1:B:113:TYR:HA	1.76	0.51
1:A:104:LEU:HD12	1:A:104:LEU:N	2.26	0.51
1:A:369:ALA:O	1:A:373:TYR:CD2	2.64	0.51
1:A:22:ILE:HG13	1:A:176:CYS:SG	2.51	0.51
1:B:210:LEU:C	1:B:214:LEU:HD22	2.31	0.51
1:B:326:VAL:N	1:B:327:PRO:HD2	2.25	0.51
1:B:17:PHE:CA	1:B:147:GLY:HA2	2.41	0.51
1:B:269:GLU:C	1:B:271:LEU:H	2.15	0.51
1:B:16:PHE:CZ	1:B:126:GLU:HA	2.45	0.51
1:B:99:LEU:N	1:B:99:LEU:HD23	2.26	0.51
1:B:294:LEU:O	1:B:298:ILE:HG12	2.11	0.51
1:A:128:PHE:CZ	1:A:132:VAL:HG21	2.45	0.51
1:B:281:LEU:N	1:B:281:LEU:CD2	2.70	0.51
1:B:376:ILE:CG2	1:B:376:ILE:O	2.59	0.51
1:A:242:GLN:HB3	1:A:373:TYR:HE2	1.76	0.51
1:A:261:PHE:O	1:A:264:VAL:CG1	2.56	0.51
1:A:100:GLN:C	1:A:102:ASN:H	2.15	0.51
1:B:299:MET:O	1:B:302:ARG:HB3	2.10	0.50
1:B:304:ILE:HG12	1:B:386:GLY:O	2.10	0.50
1:A:349:ILE:H	1:A:349:ILE:CD1	2.24	0.50
1:A:373:TYR:O	1:A:377:GLY:N	2.39	0.50
1:A:158:VAL:O	1:A:162:PHE:HB3	2.12	0.50
1:B:385:LEU:C	1:B:387:LEU:N	2.63	0.50
1:A:294:LEU:O	1:A:298:ILE:HG12	2.11	0.50
1:A:303:ILE:HG21	1:A:385:LEU:HD12	1.92	0.50
1:A:325:GLU:O	1:A:326:VAL:C	2.49	0.50
1:A:384:VAL:O	1:A:388:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:CA	1:A:147:GLY:HA2	2.40	0.50
1:A:317:ILE:N	1:A:317:ILE:HD12	2.26	0.50
1:A:275:ILE:HG13	1:A:276:MET:H	1.76	0.50
1:A:336:TYR:OH	1:A:400:LEU:HD11	2.10	0.50
1:B:23:MET:HG3	1:B:118:PHE:CD1	2.46	0.50
1:B:45:THR:HA	1:B:48:ILE:CG1	2.42	0.50
1:A:240:ASP:C	1:A:242:GLN:H	2.14	0.50
1:A:323:MET:HE3	1:A:326:VAL:HG21	1.93	0.50
1:A:125:VAL:O	1:A:129:ILE:HG12	2.11	0.50
1:A:22:ILE:HD11	1:A:173:GLY:O	2.11	0.50
1:B:158:VAL:O	1:B:162:PHE:HB3	2.12	0.50
1:B:100:GLN:C	1:B:102:ASN:H	2.14	0.50
1:B:317:ILE:HD12	1:B:317:ILE:N	2.26	0.50
1:A:136:SER:O	1:A:137:ASN:CB	2.59	0.50
1:B:369:ALA:HA	1:B:372:MET:HB3	1.92	0.50
1:A:33:TRP:CZ3	1:A:34:LEU:HD23	2.47	0.50
1:B:125:VAL:O	1:B:129:ILE:HG12	2.12	0.50
1:B:296:GLY:HA2	1:B:299:MET:CE	2.41	0.50
1:A:351:LEU:CD2	1:A:352:VAL:N	2.74	0.50
1:B:24:GLY:HA2	1:B:151:TRP:CE3	2.47	0.50
1:B:125:VAL:O	1:B:126:GLU:C	2.50	0.50
1:A:45:THR:HA	1:A:48:ILE:CG1	2.41	0.50
1:A:23:MET:HG3	1:A:118:PHE:CD1	2.47	0.49
1:B:116:PHE:O	1:B:121:GLY:N	2.45	0.49
1:B:67:SER:O	1:B:68:ASP:C	2.50	0.49
1:A:67:SER:O	1:A:68:ASP:C	2.50	0.49
1:B:226:SER:HB3	1:B:230:ILE:HD11	1.93	0.49
1:A:30:PHE:CB	1:A:31:PRO:HD3	2.30	0.49
1:A:334:PHE:HD2	1:A:335:LYS:HD2	1.77	0.49
1:B:333:CYS:O	1:B:337:ILE:HG13	2.12	0.49
1:B:334:PHE:HD2	1:B:335:LYS:HD2	1.77	0.49
1:A:275:ILE:O	1:A:276:MET:C	2.51	0.49
1:A:24:GLY:HA2	1:A:151:TRP:CE3	2.47	0.49
1:A:99:LEU:N	1:A:99:LEU:HD23	2.27	0.49
1:A:376:ILE:O	1:A:376:ILE:CG2	2.58	0.49
1:B:326:VAL:HB	1:B:327:PRO:CD	2.42	0.49
1:B:178:LEU:O	1:B:180:LEU:N	2.45	0.49
1:A:55:PHE:HE2	1:A:113:TYR:HA	1.78	0.49
1:B:42:LYS:HD3	1:B:42:LYS:N	2.21	0.49
1:B:242:GLN:HB3	1:B:373:TYR:HE2	1.77	0.49
1:B:275:ILE:HG13	1:B:276:MET:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:O	1:B:377:GLY:N	2.39	0.49
1:A:237:ASP:O	1:A:240:ASP:N	2.45	0.49
1:A:326:VAL:HB	1:A:327:PRO:CD	2.41	0.49
1:A:33:TRP:HH2	1:A:96:GLY:HA2	1.76	0.49
1:A:116:PHE:O	1:A:121:GLY:N	2.45	0.49
1:B:234:CYS:HB2	1:B:358:LYS:CD	2.42	0.49
1:A:178:LEU:O	1:A:180:LEU:N	2.45	0.49
1:B:278:PHE:HA	1:B:281:LEU:HD21	1.95	0.49
1:B:349:ILE:H	1:B:349:ILE:CD1	2.25	0.49
1:B:12:PHE:HE2	1:B:128:PHE:CE1	2.30	0.49
1:B:226:SER:O	1:B:230:ILE:HG13	2.13	0.49
1:B:298:ILE:O	1:B:299:MET:C	2.51	0.49
1:A:269:GLU:C	1:A:271:LEU:H	2.14	0.49
1:A:330:LEU:C	1:A:330:LEU:HD13	2.33	0.49
1:A:364:PHE:O	1:A:365:MET:C	2.50	0.49
1:B:253:THR:HB	1:B:254:GLY:H	1.45	0.49
1:B:364:PHE:O	1:B:365:MET:C	2.51	0.49
1:A:223:TRP:O	1:A:226:SER:HB2	2.13	0.49
1:A:19:TYR:HD2	1:A:20:PHE:HD1	1.60	0.49
1:A:282:ILE:O	1:A:286:ILE:N	2.46	0.49
1:B:33:TRP:HH2	1:B:96:GLY:HA2	1.77	0.48
1:A:379:GLN:NE2	1:A:379:GLN:H	2.08	0.48
1:A:175:GLY:C	1:A:177:ALA:H	2.16	0.48
1:B:345:PHE:O	1:B:347:ALA:N	2.46	0.48
1:B:33:TRP:CZ3	1:B:34:LEU:HD23	2.48	0.48
1:A:45:THR:HA	1:A:48:ILE:CD1	2.42	0.48
1:A:175:GLY:C	1:A:177:ALA:N	2.66	0.48
1:B:22:ILE:HD11	1:B:173:GLY:O	2.13	0.48
1:B:136:SER:O	1:B:137:ASN:CB	2.60	0.48
1:B:223:TRP:O	1:B:226:SER:HB2	2.13	0.48
1:B:44:ASP:C	1:B:47:ILE:HG22	2.34	0.48
1:A:235:THR:HG22	1:A:365:MET:SD	2.53	0.48
1:A:242:GLN:HB3	1:A:373:TYR:CE2	2.48	0.48
1:B:214:LEU:CD1	1:B:214:LEU:N	2.75	0.48
1:A:109:VAL:C	1:A:111:GLY:H	2.16	0.48
1:B:289:LYS:HG2	1:B:400:LEU:CD2	2.43	0.48
1:B:175:GLY:C	1:B:177:ALA:N	2.66	0.48
1:B:45:THR:HA	1:B:48:ILE:CD1	2.43	0.48
1:B:91:PHE:CG	1:B:170:PHE:CE2	3.01	0.48
1:A:298:ILE:O	1:A:299:MET:C	2.50	0.48
1:B:109:VAL:C	1:B:111:GLY:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.49	0.48
1:B:275:ILE:O	1:B:276:MET:C	2.52	0.48
1:A:214:LEU:N	1:A:214:LEU:CD1	2.77	0.48
1:B:240:ASP:C	1:B:242:GLN:H	2.16	0.48
1:A:234:CYS:HB2	1:A:358:LYS:CD	2.43	0.48
1:A:12:PHE:HD2	1:A:129:ILE:HD12	1.79	0.48
1:B:152:ALA:HA	1:B:266:THR:HG23	1.96	0.48
1:B:78:TRP:HH2	1:B:186:PHE:HE2	1.61	0.48
1:A:284:ASN:C	1:A:286:ILE:H	2.16	0.48
1:B:330:LEU:C	1:B:330:LEU:HD13	2.34	0.48
1:B:99:LEU:O	1:B:102:ASN:N	2.47	0.48
1:A:298:ILE:HG22	1:A:299:MET:N	2.28	0.48
1:A:388:VAL:HG13	1:A:389:ALA:N	2.29	0.48
1:B:62:LEU:HD12	1:B:62:LEU:N	2.26	0.48
1:B:234:CYS:SG	1:B:361:ALA:CB	3.02	0.48
1:A:12:PHE:HE2	1:A:128:PHE:CE1	2.30	0.48
1:B:150:GLY:O	1:B:154:CYS:CB	2.62	0.48
1:B:288:GLY:O	1:B:292:LEU:HB2	2.14	0.48
1:A:244:ALA:O	1:A:245:ASN:C	2.51	0.47
1:B:282:ILE:O	1:B:286:ILE:N	2.47	0.47
1:B:42:LYS:HG2	1:B:374:GLU:HB2	1.95	0.47
1:A:288:GLY:O	1:A:292:LEU:HB2	2.14	0.47
1:B:229:VAL:O	1:B:230:ILE:O	2.32	0.47
1:B:242:GLN:HB3	1:B:373:TYR:CE2	2.48	0.47
1:A:234:CYS:SG	1:A:361:ALA:CB	3.03	0.47
1:B:228:TYR:O	1:B:229:VAL:C	2.52	0.47
1:A:327:PRO:HG2	1:A:328:PHE:H	1.79	0.47
1:A:125:VAL:O	1:A:126:GLU:C	2.50	0.47
1:A:282:ILE:HG22	1:A:283:ILE:N	2.30	0.47
1:B:325:GLU:O	1:B:326:VAL:C	2.51	0.47
1:B:23:MET:HA	1:B:118:PHE:CE1	2.50	0.47
1:B:289:LYS:O	1:B:293:LEU:HD13	2.15	0.47
1:B:44:ASP:HB3	1:B:104:LEU:HD21	1.95	0.47
1:A:226:SER:HB3	1:A:230:ILE:HD11	1.95	0.47
1:A:162:PHE:CD2	1:A:163:THR:N	2.83	0.47
1:A:62:LEU:N	1:A:62:LEU:HD12	2.26	0.47
1:A:333:CYS:O	1:A:337:ILE:HG13	2.15	0.47
1:A:234:CYS:N	1:A:358:LYS:NZ	2.62	0.47
1:A:42:LYS:HD3	1:A:42:LYS:N	2.26	0.47
1:B:214:LEU:HD13	1:B:214:LEU:N	2.28	0.47
1:A:99:LEU:CD2	1:A:99:LEU:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:HG13	1:B:389:ALA:N	2.30	0.47
1:B:34:LEU:HD13	1:B:45:THR:HG22	1.97	0.47
1:B:234:CYS:N	1:B:358:LYS:NZ	2.63	0.47
1:A:229:VAL:O	1:A:230:ILE:O	2.33	0.47
1:A:306:SER:HB3	1:A:382:TYR:CE2	2.50	0.47
1:A:44:ASP:HB3	1:A:104:LEU:HD21	1.96	0.47
1:A:91:PHE:HA	1:A:95:PHE:HB3	1.95	0.47
1:A:260:VAL:O	1:A:260:VAL:HG12	2.14	0.47
1:A:304:ILE:HG12	1:A:386:GLY:O	2.14	0.47
1:A:154:CYS:SG	1:A:158:VAL:CG1	3.03	0.47
1:B:19:TYR:HD2	1:B:20:PHE:HD1	1.62	0.47
1:A:278:PHE:HA	1:A:281:LEU:HD21	1.97	0.47
1:B:281:LEU:O	1:B:285:ARG:CB	2.62	0.47
1:A:214:LEU:N	1:A:214:LEU:HD13	2.30	0.47
1:A:109:VAL:O	1:A:113:TYR:HB2	2.14	0.47
1:B:12:PHE:HD2	1:B:129:ILE:HD12	1.79	0.47
1:B:162:PHE:CD2	1:B:163:THR:N	2.83	0.47
1:A:78:TRP:HH2	1:A:186:PHE:HE2	1.61	0.47
1:B:222:LEU:HG	1:B:223:TRP:N	2.30	0.47
1:A:208:PHE:CE2	1:A:348:THR:HG22	2.49	0.47
1:A:17:PHE:HB2	1:A:146:PHE:O	2.14	0.47
1:B:175:GLY:C	1:B:177:ALA:H	2.16	0.47
1:B:298:ILE:HG22	1:B:299:MET:N	2.30	0.47
1:A:366:SER:O	1:A:367:VAL:C	2.53	0.47
1:B:84:LEU:HD11	1:B:118:PHE:CE2	2.50	0.47
1:B:284:ASN:C	1:B:286:ILE:H	2.18	0.47
1:B:327:PRO:HG2	1:B:328:PHE:H	1.80	0.47
1:B:306:SER:HB3	1:B:382:TYR:CE2	2.51	0.47
1:A:237:ASP:O	1:A:238:VAL:C	2.53	0.47
1:A:99:LEU:O	1:A:102:ASN:N	2.48	0.47
1:B:226:SER:C	1:B:230:ILE:HD12	2.36	0.46
1:B:233:SER:O	1:B:236:TYR:N	2.48	0.46
1:B:245:ASN:H	1:B:245:ASN:ND2	2.13	0.46
1:B:260:VAL:HG12	1:B:260:VAL:O	2.15	0.46
1:A:33:TRP:HE3	1:A:34:LEU:HD23	1.78	0.46
1:A:52:ILE:HA	1:A:112:ILE:HG21	1.97	0.46
1:A:84:LEU:HD11	1:A:118:PHE:CE2	2.49	0.46
1:A:279:ALA:O	1:A:280:PRO:C	2.52	0.46
1:B:224:PHE:N	1:B:224:PHE:CD1	2.84	0.46
1:B:232:VAL:O	1:B:236:TYR:HB3	2.15	0.46
1:B:366:SER:O	1:B:369:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ALA:HB2	1:B:366:SER:OG	2.15	0.46
1:A:150:GLY:O	1:A:154:CYS:CB	2.63	0.46
1:B:264:VAL:O	1:B:265:THR:C	2.53	0.46
1:A:42:LYS:HG2	1:A:374:GLU:HB2	1.96	0.46
1:B:57:LEU:HD22	1:B:58:LEU:HG	1.97	0.46
1:B:216:LEU:O	1:B:219:GLN:HB2	2.16	0.46
1:B:91:PHE:HA	1:B:95:PHE:HB3	1.96	0.46
1:B:282:ILE:HG22	1:B:283:ILE:N	2.29	0.46
1:B:409:LEU:C	1:B:409:LEU:HD12	2.36	0.46
1:B:244:ALA:O	1:B:245:ASN:C	2.53	0.46
1:B:232:VAL:HG11	1:B:299:MET:HE3	1.96	0.46
1:B:279:ALA:HB3	1:B:280:PRO:CD	2.42	0.46
1:B:279:ALA:O	1:B:280:PRO:C	2.53	0.46
1:A:409:LEU:HD12	1:A:409:LEU:C	2.36	0.46
1:B:109:VAL:O	1:B:113:TYR:HB2	2.16	0.46
1:A:223:TRP:CE3	1:A:223:TRP:HA	2.51	0.46
1:A:44:ASP:C	1:A:47:ILE:HG22	2.35	0.46
1:A:52:ILE:HG12	1:A:112:ILE:CG2	2.40	0.46
1:A:91:PHE:CG	1:A:170:PHE:CE2	3.04	0.46
1:A:124:ALA:O	1:A:127:ALA:HB3	2.16	0.46
1:A:154:CYS:O	1:A:155:ALA:C	2.54	0.46
1:B:237:ASP:O	1:B:238:VAL:C	2.54	0.46
1:B:33:TRP:HE3	1:B:34:LEU:HD23	1.80	0.46
1:A:320:THR:C	1:A:322:HIS:N	2.66	0.46
1:A:245:ASN:H	1:A:245:ASN:ND2	2.14	0.46
1:B:124:ALA:O	1:B:127:ALA:HB3	2.16	0.46
1:B:66:LEU:HG	1:B:67:SER:N	2.31	0.46
1:B:149:VAL:HG22	1:B:149:VAL:O	2.16	0.46
1:B:52:ILE:HA	1:B:112:ILE:HG21	1.98	0.46
1:A:295:ALA:O	1:A:299:MET:HG3	2.15	0.46
1:A:18:PHE:CG	1:A:180:LEU:HD13	2.50	0.46
1:B:12:PHE:CD1	1:B:12:PHE:N	2.82	0.46
1:A:224:PHE:CD1	1:A:224:PHE:N	2.83	0.46
1:A:358:LYS:HA	1:A:358:LYS:HD3	1.73	0.46
1:A:366:SER:O	1:A:369:ALA:N	2.49	0.46
1:B:57:LEU:HB2	1:B:359:GLN:HB2	1.98	0.46
1:B:29:PHE:CA	1:B:261:PHE:CZ	2.89	0.45
1:B:30:PHE:CB	1:B:31:PRO:HD3	2.28	0.45
1:B:91:PHE:CD1	1:B:170:PHE:HE2	2.34	0.45
1:A:228:TYR:O	1:A:229:VAL:C	2.54	0.45
1:A:349:ILE:O	1:A:353:CYS:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:N	1:A:12:PHE:CD1	2.84	0.45
1:A:264:VAL:HG22	1:A:265:THR:N	2.31	0.45
1:A:23:MET:HA	1:A:118:PHE:CE1	2.51	0.45
1:B:122:ALA:O	1:B:126:GLU:N	2.41	0.45
1:B:16:PHE:CE2	1:B:144:ARG:HD3	2.51	0.45
1:B:223:TRP:HE3	1:B:223:TRP:HA	1.81	0.45
1:B:251:PHE:CG	1:B:257:GLY:HA2	2.51	0.45
1:B:264:VAL:HG22	1:B:265:THR:N	2.31	0.45
1:A:319:LYS:O	1:A:322:HIS:CB	2.65	0.45
1:A:34:LEU:HD13	1:A:45:THR:HG22	1.97	0.45
1:A:367:VAL:CG1	1:A:368:LEU:N	2.79	0.45
1:B:72:LEU:O	1:B:74:LYS:NZ	2.49	0.45
1:B:227:LEU:N	1:B:230:ILE:HD12	2.32	0.45
1:B:26:TYR:CD1	1:B:27:PHE:HB2	2.51	0.45
1:A:395:ILE:C	1:A:397:VAL:H	2.18	0.45
1:A:117:CYS:C	1:A:121:GLY:HA3	2.36	0.45
1:A:281:LEU:O	1:A:285:ARG:CB	2.64	0.45
1:B:199:ASN:HD22	1:B:199:ASN:C	2.19	0.45
1:B:367:VAL:CG1	1:B:368:LEU:N	2.79	0.45
1:A:30:PHE:O	1:A:33:TRP:HB3	2.16	0.45
1:A:329:LEU:O	1:A:330:LEU:C	2.55	0.45
1:A:344:ARG:HH11	1:A:344:ARG:HG3	1.80	0.45
1:A:122:ALA:O	1:A:126:GLU:N	2.41	0.45
1:A:13:GLY:HA3	1:A:146:PHE:HD2	1.82	0.45
1:B:353:CYS:O	1:B:357:PHE:HB2	2.16	0.45
1:A:149:VAL:O	1:A:149:VAL:HG22	2.17	0.45
1:A:269:GLU:C	1:A:271:LEU:N	2.69	0.45
1:A:27:PHE:HB3	1:A:28:PRO:CD	2.47	0.45
1:A:57:LEU:HD11	1:A:360:LEU:HB2	1.99	0.45
1:A:154:CYS:O	1:A:157:ILE:N	2.48	0.45
1:B:329:LEU:O	1:B:330:LEU:C	2.54	0.45
1:B:395:ILE:C	1:B:397:VAL:H	2.19	0.45
1:B:52:ILE:HG12	1:B:112:ILE:CG2	2.42	0.45
1:A:289:LYS:HG2	1:A:400:LEU:CD2	2.45	0.45
1:B:344:ARG:HH11	1:B:344:ARG:HG3	1.81	0.45
1:B:154:CYS:O	1:B:155:ALA:C	2.55	0.45
1:A:149:VAL:O	1:A:152:ALA:HB3	2.17	0.45
1:B:26:TYR:HB2	1:B:87:PHE:CZ	2.52	0.45
1:B:49:PHE:HA	1:B:52:ILE:HG13	1.99	0.45
1:A:353:CYS:O	1:A:357:PHE:HB2	2.16	0.45
1:B:349:ILE:O	1:B:353:CYS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:H	1:B:99:LEU:CD2	2.25	0.45
1:B:243:PHE:CE2	1:B:247:PHE:HB2	2.51	0.45
1:B:289:LYS:HZ2	1:B:402:GLY:HA2	1.82	0.45
1:B:91:PHE:CG	1:B:170:PHE:HE2	2.34	0.45
1:A:253:THR:HB	1:A:254:GLY:H	1.45	0.45
1:A:26:TYR:HB2	1:A:87:PHE:CZ	2.52	0.45
1:B:9:PHE:CD2	1:B:10:TRP:HE3	2.32	0.45
1:B:234:CYS:O	1:B:236:TYR:N	2.50	0.45
1:B:246:PHE:CB	1:B:378:PHE:HD2	2.07	0.45
1:A:223:TRP:HE3	1:A:223:TRP:HA	1.82	0.45
1:A:347:ALA:O	1:A:351:LEU:N	2.45	0.45
1:B:334:PHE:HD1	1:B:350:TYR:OH	2.00	0.45
1:B:354:PHE:CD1	1:B:354:PHE:N	2.85	0.45
1:B:398:PHE:O	1:B:400:LEU:N	2.49	0.44
1:A:334:PHE:HD1	1:A:350:TYR:OH	2.00	0.44
1:A:127:ALA:O	1:A:130:GLU:HB3	2.17	0.44
1:A:85:VAL:O	1:A:85:VAL:HG12	2.17	0.44
1:B:279:ALA:O	1:B:282:ILE:HB	2.17	0.44
1:B:374:GLU:O	1:B:374:GLU:HG2	2.17	0.44
1:B:246:PHE:HZ	1:B:309:ALA:HB2	1.83	0.44
1:A:251:PHE:CG	1:A:257:GLY:HA2	2.53	0.44
1:B:244:ALA:C	1:B:246:PHE:N	2.70	0.44
1:B:319:LYS:O	1:B:322:HIS:CB	2.63	0.44
1:A:222:LEU:HG	1:A:223:TRP:N	2.30	0.44
1:A:299:MET:O	1:A:302:ARG:N	2.45	0.44
1:A:84:LEU:C	1:A:86:MET:N	2.71	0.44
1:A:279:ALA:HB3	1:A:280:PRO:CD	2.43	0.44
1:B:17:PHE:HB2	1:B:146:PHE:O	2.16	0.44
1:B:75:TYR:O	1:B:76:LEU:C	2.55	0.44
1:B:302:ARG:CZ	1:B:318:LEU:O	2.66	0.44
1:A:264:VAL:O	1:A:265:THR:C	2.54	0.44
1:A:289:LYS:O	1:A:293:LEU:HD13	2.17	0.44
1:A:57:LEU:HD12	1:A:360:LEU:N	2.33	0.44
1:A:246:PHE:HZ	1:A:309:ALA:HB2	1.82	0.44
1:A:16:PHE:CE2	1:A:144:ARG:HD3	2.53	0.44
1:A:9:PHE:CD2	1:A:10:TRP:HE3	2.33	0.44
1:A:66:LEU:HG	1:A:67:SER:N	2.32	0.44
1:B:3:TYR:HB3	1:B:138:PHE:CD2	2.52	0.44
1:B:299:MET:HG2	1:B:325:GLU:HG3	2.00	0.44
1:A:233:SER:O	1:A:236:TYR:N	2.49	0.44
1:A:259:ARG:O	1:A:261:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PHE:O	1:A:400:LEU:N	2.50	0.44
1:A:57:LEU:HD22	1:A:58:LEU:HG	2.00	0.44
1:A:12:PHE:CE2	1:A:128:PHE:HE1	2.36	0.44
1:A:109:VAL:C	1:A:111:GLY:N	2.71	0.44
1:B:259:ARG:O	1:B:261:PHE:N	2.50	0.44
1:B:269:GLU:C	1:B:271:LEU:N	2.69	0.44
1:B:387:LEU:O	1:B:390:LEU:N	2.50	0.44
1:A:240:ASP:C	1:A:242:GLN:N	2.70	0.44
1:B:7:THR:CG2	1:B:8:ASN:H	2.25	0.44
1:B:109:VAL:C	1:B:111:GLY:N	2.71	0.44
1:B:33:TRP:HA	1:B:37:ILE:HB	2.00	0.44
1:A:209:SER:O	1:A:212:LEU:HB3	2.17	0.44
1:B:57:LEU:HB2	1:B:359:GLN:CB	2.48	0.44
1:B:320:THR:C	1:B:322:HIS:N	2.68	0.44
1:A:275:ILE:HD12	1:A:327:PRO:HB3	2.00	0.44
1:A:45:THR:CG2	1:A:48:ILE:HD12	2.38	0.44
1:B:209:SER:O	1:B:212:LEU:HB3	2.17	0.44
1:A:7:THR:O	1:A:10:TRP:N	2.50	0.44
1:A:75:TYR:O	1:A:76:LEU:C	2.56	0.44
1:A:64:GLY:O	1:A:66:LEU:N	2.50	0.44
1:B:263:TYR:H	1:B:263:TYR:HD1	1.65	0.44
1:A:216:LEU:O	1:A:219:GLN:HB2	2.17	0.44
1:A:246:PHE:CD1	1:A:247:PHE:N	2.86	0.44
1:B:78:TRP:HZ2	1:B:185:PHE:HB3	1.82	0.44
1:B:149:VAL:O	1:B:152:ALA:HB3	2.17	0.44
1:B:275:ILE:HD12	1:B:327:PRO:HB3	2.00	0.43
1:B:392:PHE:O	1:B:395:ILE:HG22	2.18	0.43
1:A:50:ALA:HB1	1:A:363:ILE:O	2.18	0.43
1:A:175:GLY:O	1:A:178:LEU:N	2.51	0.43
1:B:416:VAL:O	1:B:417:ALA:HB2	2.17	0.43
1:B:117:CYS:C	1:B:121:GLY:HA3	2.37	0.43
1:A:60:GLN:HB2	1:A:60:GLN:HE21	1.60	0.43
1:A:26:TYR:CD1	1:A:27:PHE:HB2	2.53	0.43
1:A:299:MET:HG2	1:A:325:GLU:HG3	2.00	0.43
1:A:374:GLU:HG2	1:A:374:GLU:O	2.18	0.43
1:A:387:LEU:O	1:A:390:LEU:N	2.51	0.43
1:B:84:LEU:C	1:B:86:MET:N	2.70	0.43
1:A:279:ALA:O	1:A:282:ILE:HB	2.18	0.43
1:B:337:ILE:HB	1:B:338:THR:H	1.60	0.43
1:B:275:ILE:HD13	1:B:327:PRO:CB	2.48	0.43
1:B:395:ILE:HG12	1:B:399:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD13	1:A:327:PRO:CB	2.48	0.43
1:A:344:ARG:NH1	1:A:344:ARG:HG3	2.33	0.43
1:A:345:PHE:O	1:A:346:SER:C	2.55	0.43
1:A:243:PHE:CE2	1:A:247:PHE:HB2	2.53	0.43
1:B:85:VAL:O	1:B:85:VAL:HG12	2.17	0.43
1:A:281:LEU:N	1:A:281:LEU:CD2	2.69	0.43
1:B:154:CYS:O	1:B:157:ILE:N	2.49	0.43
1:B:101:TYR:HD2	1:B:101:TYR:HA	1.65	0.43
1:B:246:PHE:CD1	1:B:247:PHE:N	2.86	0.43
1:B:27:PHE:HB3	1:B:28:PRO:CD	2.48	0.43
1:B:395:ILE:C	1:B:397:VAL:N	2.72	0.43
1:A:169:VAL:CG2	1:A:170:PHE:H	2.30	0.43
1:A:230:ILE:HA	1:A:358:LYS:HE2	2.00	0.43
1:B:154:CYS:SG	1:B:158:VAL:CG1	3.06	0.43
1:B:299:MET:O	1:B:302:ARG:N	2.44	0.43
1:B:358:LYS:O	1:B:361:ALA:N	2.51	0.43
1:A:226:SER:C	1:A:230:ILE:HD12	2.39	0.43
1:A:395:ILE:HG12	1:A:399:THR:OG1	2.19	0.43
1:A:91:PHE:CD1	1:A:170:PHE:HE2	2.37	0.43
1:B:22:ILE:HG13	1:B:176:CYS:SG	2.58	0.43
1:B:210:LEU:O	1:B:214:LEU:HD22	2.18	0.43
1:A:416:VAL:O	1:A:417:ALA:HB2	2.18	0.43
1:B:16:PHE:HZ	1:B:126:GLU:HA	1.82	0.43
1:A:354:PHE:N	1:A:354:PHE:CD1	2.86	0.43
1:B:366:SER:O	1:B:367:VAL:C	2.56	0.43
1:A:295:ALA:HB2	1:A:328:PHE:CB	2.48	0.43
1:A:33:TRP:HA	1:A:37:ILE:HB	2.01	0.43
1:A:244:ALA:C	1:A:246:PHE:N	2.69	0.43
1:B:18:PHE:CG	1:B:180:LEU:HD13	2.53	0.43
1:B:19:TYR:C	1:B:19:TYR:CD2	2.91	0.43
1:A:283:ILE:HD13	1:A:283:ILE:H	1.84	0.43
1:B:211:LYS:O	1:B:214:LEU:HB2	2.18	0.43
1:B:7:THR:O	1:B:10:TRP:N	2.51	0.43
1:B:121:GLY:C	1:B:123:PRO:HD2	2.38	0.43
1:B:13:GLY:HA3	1:B:146:PHE:HD2	1.83	0.43
1:A:199:ASN:HD22	1:A:199:ASN:C	2.20	0.43
1:B:354:PHE:HD1	1:B:354:PHE:H	1.66	0.43
1:A:3:TYR:HB3	1:A:138:PHE:CD2	2.53	0.43
1:A:16:PHE:HZ	1:A:126:GLU:HA	1.83	0.43
1:A:64:GLY:C	1:A:66:LEU:H	2.22	0.43
1:B:336:TYR:CZ	1:B:400:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:CA	1:A:261:PHE:CZ	2.89	0.43
1:A:395:ILE:C	1:A:397:VAL:N	2.72	0.43
1:A:19:TYR:HD2	1:A:20:PHE:CD1	2.37	0.43
1:A:72:LEU:O	1:A:74:LYS:NZ	2.51	0.43
1:B:229:VAL:HG12	1:B:358:LYS:CE	2.48	0.43
1:B:295:ALA:O	1:B:299:MET:HG3	2.18	0.43
1:B:74:LYS:N	1:B:74:LYS:HD2	2.34	0.43
1:B:345:PHE:HB3	1:B:349:ILE:CD1	2.47	0.43
1:B:62:LEU:CD1	1:B:62:LEU:H	2.26	0.43
1:A:358:LYS:O	1:A:361:ALA:N	2.51	0.43
1:A:91:PHE:CE1	1:A:95:PHE:HD2	2.37	0.43
1:A:154:CYS:SG	1:A:158:VAL:HG13	2.58	0.43
1:A:32:ILE:HG22	1:A:33:TRP:N	2.33	0.42
1:A:49:PHE:HA	1:A:52:ILE:HG13	2.01	0.42
1:A:246:PHE:HD2	1:A:378:PHE:HB3	1.83	0.42
1:B:169:VAL:CG2	1:B:170:PHE:H	2.32	0.42
1:B:169:VAL:CG2	1:B:170:PHE:N	2.81	0.42
1:B:246:PHE:HD2	1:B:378:PHE:HB3	1.83	0.42
1:A:232:VAL:O	1:A:236:TYR:HB3	2.18	0.42
1:A:263:TYR:HD1	1:A:263:TYR:H	1.66	0.42
1:A:19:TYR:CD2	1:A:19:TYR:C	2.92	0.42
1:B:211:LYS:N	1:B:214:LEU:HD22	2.33	0.42
1:B:74:LYS:CE	1:B:190:ASP:HB2	2.49	0.42
1:A:408:LEU:O	1:A:409:LEU:HB3	2.20	0.42
1:A:302:ARG:CZ	1:A:318:LEU:O	2.68	0.42
1:B:344:ARG:NH1	1:B:344:ARG:HG3	2.33	0.42
1:B:345:PHE:O	1:B:346:SER:C	2.57	0.42
1:B:243:PHE:O	1:B:244:ALA:C	2.58	0.42
1:A:233:SER:O	1:A:234:CYS:C	2.57	0.42
1:A:230:ILE:C	1:A:234:CYS:HB3	2.37	0.42
1:A:302:ARG:HG2	1:A:302:ARG:O	2.19	0.42
1:B:278:PHE:O	1:B:281:LEU:HD23	2.20	0.42
1:B:344:ARG:NE	1:B:345:PHE:HE1	2.18	0.42
1:B:127:ALA:O	1:B:130:GLU:HB3	2.18	0.42
1:B:255:GLU:O	1:B:259:ARG:CB	2.66	0.42
1:B:30:PHE:CB	1:B:31:PRO:CD	2.93	0.42
1:B:19:TYR:HD2	1:B:20:PHE:CD1	2.38	0.42
1:B:278:PHE:HA	1:B:281:LEU:HD23	2.00	0.42
1:B:152:ALA:O	1:B:153:LEU:C	2.58	0.42
1:B:240:ASP:C	1:B:242:GLN:N	2.72	0.42
1:A:364:PHE:O	1:A:366:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:C	1:A:123:PRO:HD2	2.40	0.42
1:A:17:PHE:O	1:A:21:PHE:HB2	2.19	0.42
1:B:23:MET:HA	1:B:118:PHE:CZ	2.55	0.42
1:A:62:LEU:H	1:A:62:LEU:CD1	2.26	0.42
1:B:11:MET:C	1:B:12:PHE:CD1	2.93	0.42
1:B:233:SER:O	1:B:234:CYS:C	2.58	0.42
1:B:275:ILE:HD13	1:B:327:PRO:CD	2.49	0.42
1:B:64:GLY:O	1:B:66:LEU:N	2.51	0.42
1:B:319:LYS:C	1:B:321:LEU:N	2.73	0.42
1:B:91:PHE:CE1	1:B:95:PHE:HD2	2.38	0.42
1:A:255:GLU:O	1:A:259:ARG:CB	2.66	0.42
1:A:289:LYS:HD3	1:A:289:LYS:C	2.40	0.42
1:A:16:PHE:HB3	1:A:147:GLY:HA3	2.01	0.42
1:A:74:LYS:CE	1:A:190:ASP:HB2	2.49	0.42
1:B:9:PHE:HD2	1:B:10:TRP:CE3	2.34	0.42
1:A:75:TYR:O	1:A:77:LEU:N	2.53	0.42
1:B:408:LEU:O	1:B:409:LEU:HB3	2.20	0.42
1:B:385:LEU:HG	1:B:385:LEU:H	1.44	0.42
1:B:26:TYR:HB2	1:B:87:PHE:CE1	2.55	0.42
1:A:227:LEU:N	1:A:230:ILE:HD12	2.35	0.42
1:B:75:TYR:O	1:B:77:LEU:N	2.53	0.42
1:B:88:ALA:N	1:B:89:PRO:CD	2.83	0.42
1:A:91:PHE:CG	1:A:170:PHE:HE2	2.37	0.42
1:A:42:LYS:O	1:A:45:THR:OG1	2.34	0.42
1:A:144:ARG:C	1:A:146:PHE:N	2.73	0.42
1:B:144:ARG:C	1:B:146:PHE:N	2.73	0.42
1:A:186:PHE:N	1:A:186:PHE:CD2	2.87	0.42
1:B:260:VAL:O	1:B:264:VAL:HB	2.20	0.41
1:B:302:ARG:O	1:B:302:ARG:HG2	2.20	0.41
1:B:378:PHE:O	1:B:382:TYR:CG	2.73	0.41
1:A:234:CYS:O	1:A:236:TYR:N	2.52	0.41
1:A:349:ILE:O	1:A:353:CYS:HB3	2.20	0.41
1:A:369:ALA:HA	1:A:372:MET:HB2	2.01	0.41
1:A:278:PHE:HA	1:A:281:LEU:HD23	2.01	0.41
1:B:122:ALA:O	1:B:126:GLU:HG3	2.20	0.41
1:B:17:PHE:O	1:B:21:PHE:HB2	2.19	0.41
1:A:169:VAL:CG2	1:A:170:PHE:N	2.78	0.41
1:A:275:ILE:HD13	1:A:327:PRO:CD	2.50	0.41
1:A:41:SER:O	1:A:44:ASP:HB2	2.21	0.41
1:B:286:ILE:CG2	1:B:291:ALA:HB2	2.50	0.41
1:B:264:VAL:CG1	1:B:265:THR:N	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:HB	1:B:386:GLY:CA	2.48	0.41
1:B:319:LYS:C	1:B:321:LEU:H	2.23	0.41
1:B:394:LEU:O	1:B:397:VAL:CG2	2.67	0.41
1:A:27:PHE:O	1:A:28:PRO:C	2.58	0.41
1:A:337:ILE:HG13	1:A:337:ILE:H	1.48	0.41
1:A:11:MET:HG2	1:A:187:ALA:O	2.20	0.41
1:A:151:TRP:O	1:A:155:ALA:N	2.53	0.41
1:B:2:TYR:HE2	1:B:137:ASN:OD1	2.03	0.41
1:B:1:MET:CG	1:B:4:LEU:HD22	2.50	0.41
1:B:289:LYS:C	1:B:289:LYS:HD3	2.40	0.41
1:A:229:VAL:HG12	1:A:358:LYS:CE	2.49	0.41
1:A:336:TYR:CZ	1:A:400:LEU:HD11	2.55	0.41
1:B:64:GLY:C	1:B:66:LEU:H	2.24	0.41
1:B:336:TYR:OH	1:B:400:LEU:CD1	2.69	0.41
1:A:94:ILE:O	1:A:98:LEU:HB2	2.20	0.41
1:A:246:PHE:CZ	1:A:309:ALA:CB	3.01	0.41
1:A:17:PHE:CE1	1:A:150:GLY:CA	3.04	0.41
1:B:175:GLY:O	1:B:178:LEU:N	2.54	0.41
1:A:392:PHE:O	1:A:395:ILE:HG22	2.21	0.41
1:A:247:PHE:CD1	1:A:315:VAL:HG23	2.55	0.41
1:A:286:ILE:CG2	1:A:291:ALA:HB2	2.50	0.41
1:B:32:ILE:HG22	1:B:33:TRP:N	2.35	0.41
1:A:52:ILE:CB	1:A:112:ILE:HG21	2.51	0.41
1:A:19:TYR:CD2	1:A:20:PHE:N	2.88	0.41
1:A:84:LEU:C	1:A:86:MET:H	2.24	0.41
1:A:15:PHE:HB2	1:A:184:LEU:HD13	2.03	0.41
1:A:43:SER:HB2	1:A:371:ASN:OD1	2.21	0.41
1:B:247:PHE:CD1	1:B:315:VAL:HG23	2.56	0.41
1:A:263:TYR:O	1:A:264:VAL:O	2.39	0.41
1:A:394:LEU:O	1:A:397:VAL:CG2	2.67	0.41
1:B:186:PHE:CD2	1:B:186:PHE:N	2.89	0.41
1:A:298:ILE:HA	1:A:298:ILE:HD13	1.83	0.41
1:A:88:ALA:N	1:A:89:PRO:CD	2.84	0.41
1:A:246:PHE:CB	1:A:378:PHE:HD2	2.08	0.41
1:B:283:ILE:HD13	1:B:283:ILE:H	1.85	0.41
1:A:211:LYS:O	1:A:214:LEU:HB2	2.21	0.41
1:B:154:CYS:SG	1:B:158:VAL:HG13	2.61	0.41
1:B:11:MET:HG2	1:B:187:ALA:O	2.21	0.41
1:B:16:PHE:HB3	1:B:147:GLY:HA3	2.02	0.41
1:A:38:ASN:O	1:A:39:HIS:C	2.59	0.41
1:B:317:ILE:CD1	1:B:317:ILE:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:O	1:A:153:LEU:C	2.59	0.41
1:A:239:PHE:CE2	1:A:243:PHE:HD1	2.39	0.41
1:B:84:LEU:C	1:B:86:MET:H	2.23	0.41
1:A:7:THR:CG2	1:A:8:ASN:H	2.24	0.41
1:B:12:PHE:CE2	1:B:128:PHE:HE1	2.36	0.41
1:A:1:MET:CG	1:A:4:LEU:HD22	2.50	0.41
1:B:230:ILE:H	1:B:230:ILE:HG13	1.70	0.40
1:B:246:PHE:CZ	1:B:309:ALA:CB	3.01	0.40
1:B:369:ALA:HA	1:B:372:MET:HB2	2.03	0.40
1:A:234:CYS:N	1:A:358:LYS:HZ3	2.19	0.40
1:B:19:TYR:CD2	1:B:20:PHE:N	2.89	0.40
1:B:99:LEU:C	1:B:101:TYR:N	2.74	0.40
1:B:27:PHE:O	1:B:28:PRO:C	2.58	0.40
1:B:94:ILE:O	1:B:98:LEU:HB2	2.22	0.40
1:A:345:PHE:HB3	1:A:349:ILE:CD1	2.48	0.40
1:B:349:ILE:O	1:B:353:CYS:HB3	2.20	0.40
1:A:2:TYR:HE2	1:A:137:ASN:OD1	2.04	0.40
1:B:30:PHE:O	1:B:33:TRP:HB3	2.21	0.40
1:B:44:ASP:O	1:B:47:ILE:CG2	2.68	0.40
1:A:42:LYS:O	1:A:44:ASP:N	2.53	0.40
1:A:23:MET:HA	1:A:118:PHE:CZ	2.57	0.40
1:A:278:PHE:O	1:A:281:LEU:HD23	2.21	0.40
1:B:337:ILE:H	1:B:337:ILE:HG13	1.47	0.40
1:B:127:ALA:O	1:B:128:PHE:C	2.59	0.40
1:B:297:THR:O	1:B:301:VAL:HG23	2.21	0.40
1:A:127:ALA:O	1:A:128:PHE:C	2.60	0.40
1:B:52:ILE:CG2	1:B:112:ILE:HG21	2.50	0.40
1:B:45:THR:CG2	1:B:48:ILE:HD12	2.38	0.40
1:A:345:PHE:C	1:A:349:ILE:HD13	2.41	0.40
1:A:11:MET:C	1:A:12:PHE:CD1	2.95	0.40
1:B:19:TYR:O	1:B:22:ILE:CG2	2.60	0.40
1:A:99:LEU:CD2	1:A:107:SER:HB3	2.52	0.40
1:A:354:PHE:HD1	1:A:354:PHE:H	1.68	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%)	228 (55%)	113 (27%)	74 (18%)	0 3
1	B	415/417 (100%)	229 (55%)	111 (27%)	75 (18%)	0 3
All	All	830/834 (100%)	457 (55%)	224 (27%)	149 (18%)	0 3

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	39	HIS
1	A	70	LEU
1	A	102	ASN
1	A	105	VAL
1	A	127	ALA
1	A	137	ASN
1	A	139	GLU
1	A	152	ALA
1	A	155	ALA
1	A	178	LEU
1	A	230	ILE
1	A	234	CYS
1	A	244	ALA
1	A	245	ASN
1	A	259	ARG
1	A	264	VAL
1	A	282	ILE
1	A	283	ILE
1	A	327	PRO
1	A	328	PHE
1	A	343	VAL
1	A	346	SER
1	A	356	PHE
1	A	365	MET

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Mol	Chain	Res	Type
1	A	399	THR
1	A	402	GLY
1	A	409	LEU
1	B	36	ASP
1	B	39	HIS
1	B	70	LEU
1	B	102	ASN
1	B	105	VAL
1	B	127	ALA
1	B	137	ASN
1	B	139	GLU
1	B	152	ALA
1	B	155	ALA
1	B	178	LEU
1	B	230	ILE
1	B	234	CYS
1	B	244	ALA
1	B	245	ASN
1	B	259	ARG
1	B	264	VAL
1	B	282	ILE
1	B	283	ILE
1	B	327	PRO
1	B	328	PHE
1	B	337	ILE
1	B	343	VAL
1	B	346	SER
1	B	356	PHE
1	B	365	MET
1	B	399	THR
1	B	402	GLY
1	B	409	LEU
1	A	24	GLY
1	A	30	PHE
1	A	35	HIS
1	A	56	SER
1	A	76	LEU
1	A	91	PHE
1	A	179	ILE
1	A	231	GLY
1	A	258	THR
1	A	277	PHE

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Mol	Chain	Res	Type
1	A	309	ALA
1	A	330	LEU
1	A	337	ILE
1	A	338	THR
1	A	353	CYS
1	A	355	CYS
1	A	404	GLY
1	B	24	GLY
1	B	30	PHE
1	B	35	HIS
1	B	56	SER
1	B	76	LEU
1	B	91	PHE
1	B	179	ILE
1	B	231	GLY
1	B	258	THR
1	B	277	PHE
1	B	309	ALA
1	B	330	LEU
1	B	338	THR
1	B	353	CYS
1	B	355	CYS
1	B	404	GLY
1	A	26	TYR
1	A	193	SER
1	A	278	PHE
1	A	339	SER
1	A	340	GLN
1	A	364	PHE
1	B	26	TYR
1	B	193	SER
1	B	265	THR
1	B	278	PHE
1	B	339	SER
1	B	340	GLN
1	B	349	ILE
1	B	364	PHE
1	A	65	LEU
1	A	87	PHE
1	A	232	VAL
1	A	235	THR
1	A	265	THR

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Mol	Chain	Res	Type
1	A	276	MET
1	A	290	ASN
1	A	349	ILE
1	A	354	PHE
1	B	65	LEU
1	B	87	PHE
1	B	154	CYS
1	B	233	SER
1	B	276	MET
1	B	290	ASN
1	B	354	PHE
1	A	43	SER
1	A	154	CYS
1	A	233	SER
1	A	260	VAL
1	A	280	PRO
1	A	281	LEU
1	A	367	VAL
1	B	43	SER
1	B	232	VAL
1	B	280	PRO
1	B	281	LEU
1	B	323	MET
1	A	57	LEU
1	A	347	ALA
1	B	57	LEU
1	B	235	THR
1	B	260	VAL
1	B	347	ALA
1	B	367	VAL
1	B	229	VAL
1	A	27	PHE
1	A	229	VAL
1	A	238	VAL
1	B	238	VAL
1	A	92	ILE
1	A	416	VAL
1	B	27	PHE
1	B	416	VAL
1	B	92	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	346/346 (100%)	292 (84%)	54 (16%)	3 23
1	B	346/346 (100%)	291 (84%)	55 (16%)	3 21
All	All	692/692 (100%)	583 (84%)	109 (16%)	3 22

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	TYR
1	A	10	TRP
1	A	11	MET
1	A	16	PHE
1	A	19	TYR
1	A	26	TYR
1	A	42	LYS
1	A	59	PHE
1	A	60	GLN
1	A	83	MET
1	A	99	LEU
1	A	101	TYR
1	A	112	ILE
1	A	128	PHE
1	A	131	LYS
1	A	140	PHE
1	A	142	ARG
1	A	148	CYS
1	A	151	TRP
1	A	161	MET
1	A	162	PHE
1	A	163	THR
1	A	171	TRP
1	A	188	LYS
1	A	199	ASN
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	217	PHE
1	A	223	TRP
1	A	225	LEU
1	A	239	PHE
1	A	240	ASP
1	A	253	THR
1	A	269	GLU
1	A	275	ILE
1	A	281	LEU
1	A	289	LYS
1	A	323	MET
1	A	329	LEU
1	A	331	VAL
1	A	337	ILE
1	A	340	GLN
1	A	344	ARG
1	A	351	LEU
1	A	356	PHE
1	A	358	LYS
1	A	367	VAL
1	A	379	GLN
1	A	385	LEU
1	A	393	THR
1	A	394	LEU
1	A	408	LEU
1	A	410	ARG
1	B	1	MET
1	B	2	TYR
1	B	10	TRP
1	B	11	MET
1	B	16	PHE
1	B	19	TYR
1	B	26	TYR
1	B	42	LYS
1	B	59	PHE
1	B	60	GLN
1	B	83	MET
1	B	99	LEU
1	B	101	TYR
1	B	112	ILE
1	B	128	PHE

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Mol	Chain	Res	Type
1	B	131	LYS
1	B	140	PHE
1	B	142	ARG
1	B	148	CYS
1	B	151	TRP
1	B	161	MET
1	B	162	PHE
1	B	163	THR
1	B	171	TRP
1	B	188	LYS
1	B	199	ASN
1	B	210	LEU
1	B	214	LEU
1	B	217	PHE
1	B	223	TRP
1	B	225	LEU
1	B	239	PHE
1	B	240	ASP
1	B	253	THR
1	B	269	GLU
1	B	275	ILE
1	B	281	LEU
1	B	289	LYS
1	B	323	MET
1	B	325	GLU
1	B	329	LEU
1	B	331	VAL
1	B	337	ILE
1	B	340	GLN
1	B	344	ARG
1	B	351	LEU
1	B	356	PHE
1	B	358	LYS
1	B	367	VAL
1	B	379	GLN
1	B	385	LEU
1	B	393	THR
1	B	394	LEU
1	B	408	LEU
1	B	410	ARG

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	60	GLN
1	A	199	ASN
1	A	219	GLN
1	A	241	GLN
1	A	245	ASN
1	A	379	GLN
1	B	8	ASN
1	B	60	GLN
1	B	199	ASN
1	B	219	GLN
1	B	241	GLN
1	B	242	GLN
1	B	245	ASN
1	B	359	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	417/417 (100%)	-0.22	22 (5%)	30	21	15, 81, 164, 196	0
1	B	417/417 (100%)	-0.01	26 (6%)	24	16	21, 80, 164, 196	0
All	All	834/834 (100%)	-0.12	48 (5%)	26	18	15, 81, 164, 196	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	SER	14.8
1	B	193	SER	9.4
1	B	410	ARG	8.8
1	B	192	PRO	8.1
1	B	195	ALA	6.8
1	B	197	VAL	6.6
1	B	417	ALA	5.7
1	B	102	ASN	5.5
1	A	102	ASN	5.1
1	B	100	GLN	5.1
1	B	191	ALA	5.0
1	B	252	ALA	4.8
1	A	407	SER	4.4
1	A	190	ASP	4.3
1	A	417	ALA	4.3
1	B	190	ASP	4.2
1	A	252	ALA	4.2
1	A	194	SER	4.1
1	B	413	VAL	4.0
1	B	409	LEU	3.8
1	A	406	LEU	3.8
1	A	195	ALA	3.7
1	B	253	THR	3.7
1	B	101	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	100	GLN	3.5
1	B	201	VAL	3.5
1	A	101	TYR	3.4
1	B	285	ARG	3.2
1	A	193	SER	3.1
1	B	198	ALA	3.0
1	A	410	ARG	3.0
1	B	414	ASN	3.0
1	B	196	THR	3.0
1	A	413	VAL	2.9
1	B	286	ILE	2.8
1	A	408	LEU	2.7
1	A	202	GLY	2.6
1	A	317	ILE	2.5
1	B	202	GLY	2.5
1	A	201	VAL	2.4
1	A	409	LEU	2.4
1	A	39	HIS	2.4
1	A	253	THR	2.4
1	B	106	GLY	2.2
1	A	192	PRO	2.1
1	B	407	SER	2.1
1	A	286	ILE	2.0
1	B	411	ARG	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.