



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:11 am GMT

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

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

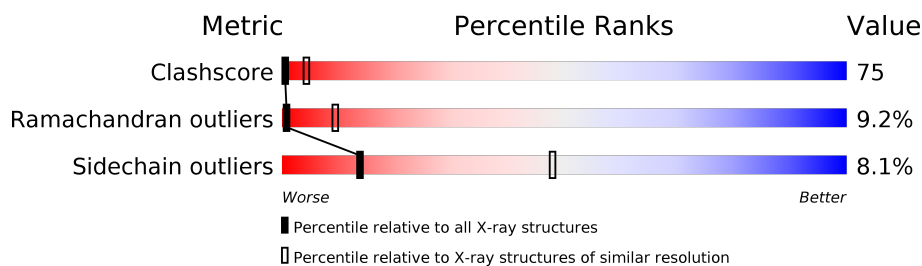
1 Overall quality at a glance

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	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	417	
1	B	417	

2 Entry composition

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:

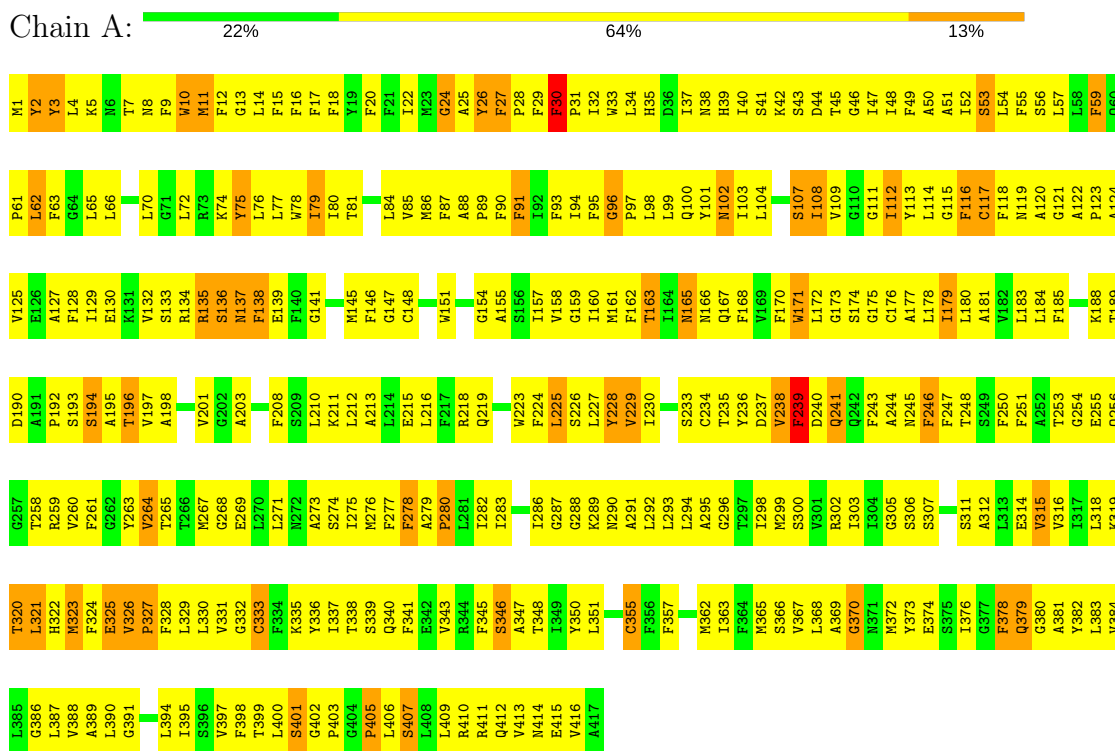
Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	ENGINEERED	UNP P02920
B	154	GLY	CYS	ENGINEERED	UNP P02920

3 Residue-property plots

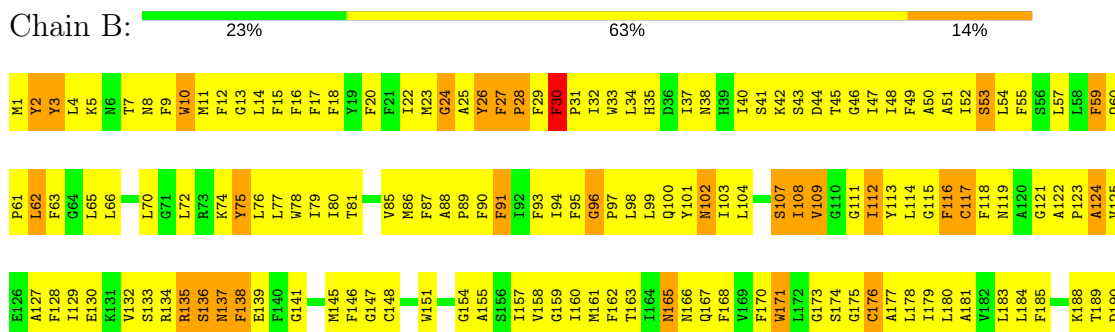
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: Lactose permease



- Molecule 1: Lactose permease



L385	M323	T258	A191
G366	G324	R259	P192
	E325	V260	S193
L390	V326	G261	S194
G391	P327	G262	A195
	F328	Y263	T196
I395	L329	V264	V197
S396	L330	T265	A198
P397	V331	T266	
F398	G332	M267	V201
T399	C333	G268	G202
L400	F334	E269	A203
S401	K335	L270	
G402	L336	L271	F208
P403	V337	M272	S209
G404	T338	A273	L210
P405	S339	S274	K211
L406	Q340	L275	L212
S407	F341	M276	L214
L408	E342	F277	A214
L409	V343	F278	E215
L410	R344	A279	L216
R411	F345	P280	F217
Q412	S346	L281	R218
V413	A347	L282	Q219
N414	L348	L283	
E415	L349	L286	W223
V416	V350	G287	F224
A417	L351	G288	L225
		K289	S226
	C355	M290	L227
	F356	A291	Y228
	F357	L292	V229
	K358	L293	L230
	Q359	L294	
	L360	A295	S233
	A361	G296	C234
	M362	T297	T235
	L363	L298	Y236
	F364	M299	D237
	K365	S300	V238
	S366	V301	F239
	V367	R302	D240
	A369	I303	Q241
	G370		Q242
	N371	S306	F243
	M372	S307	A244
	Y373		V245
	E374	S311	F246
	S375	L248	T247
	F376	E314	T248
	G377	V315	S249
	F378	V316	F250
	Q379	I317	F251
	G380	L318	A252
	A381	K319	G254
	T382	T320	G255
	L383	L321	Q256
	N384	H221	G257

4 Data and refinement statistics

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(°)	Ideal(°)
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:166:ASN:OD1	1:A:167:GLN:N	2.15	0.78
1:A:85:VAL:HG22	1:A:178:LEU:HB2	1.66	0.78
1:B:28:PRO:O	1:B:31:PRO:HD2	1.83	0.78
1:B:1:MET:O	1:B:3:TYR:N	2.15	0.78
1:A:275:ILE:HG21	1:A:327:PRO:HG3	1.66	0.78
1:A:121:GLY:HA2	1:A:124:ALA:HB3	1.65	0.78
1:A:27:PHE:HB3	1:A:28:PRO:CD	2.13	0.78
1:A:10:TRP:HE1	1:B:168:PHE:HD1	1.29	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:48:ILE:HA	1:B:108:ILE:HG23	1.65	0.76
1:B:16:PHE:HE1	1:B:129:ILE:HG21	1.50	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:166:ASN:OD1	1:B:167:GLN:N	2.19	0.75
1:B:90:PHE:CE2	1:B:114:LEU:HB3	2.22	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:121:GLY:O	1:A:124:ALA:HB3	1.86	0.74
1:A:1:MET:HB2	1:A:3:TYR:CZ	2.23	0.74
1:B:99:LEU:CD2	1:B:104:LEU:HD12	2.16	0.74
1:B:27:PHE:HB3	1:B:28:PRO:HD2	1.68	0.74
1:B:271:LEU:HD23	1:B:323:MET:HB2	1.69	0.74
1:B:87:PHE:HB3	1:B:174:SER: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:122:ALA:HB3	1:A:123:PRO:CD	2.18	0.73
1:A:44:ASP:HA	1:A:104:LEU:HD21	1.71	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:H	1:B:74:LYS:HD2	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:163:THR:HG21	1:B:255:GLU:HG3	1.71	0.72
1:B:171:TRP:CE3	1:B:171:TRP:HA	2.24	0.72
1:B:93:PHE:O	1:B:97:PRO:HG2	1.90	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: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:A:27:PHE:HB3	1:A:28: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:HA	1:B:415:GLU:OE1	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: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:90:PHE:CZ	1:A:114:LEU:HB3	2.28	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:HE3	1:B:171:TRP:HA	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:CE3	1:A:171:TRP:HA	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:48:ILE:HA	1:A:108:ILE:CG2	2.27	0.65
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.32	0.65
1:A:289:LYS:HD3	1:A:403:PRO:HG3	1.77	0.65
1:B:323:MET:N	1:B:323:MET:SD	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:292:LEU:HD21	1:B:333:CYS:N	2.13	0.63
1:B:283:ILE:HG13	1:B:331:VAL:CG1	2.27	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:161:MET:HB3	1:B:168:PHE:HE2	1.64	0.63
1:B:16:PHE:HB3	1:B:147:GLY:CA	2.29	0.63
1:A:34:LEU:HD13	1:A:40:ILE:CD1	2.24	0.63
1:A:16:PHE:CD1	1:A:129:ILE:HD12	2.34	0.62
1:A:16:PHE:HB3	1:A:147:GLY:CA	2.29	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:319:LYS:O	1:A:320:THR:C	2.38	0.62
1:A:292:LEU:HD21	1:A:333:CYS:N	2.14	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:323:MET:O	1:B:327:PRO:HD2	1.99	0.62
1:B:90:PHE:CE2	1:B:95:PHE:HE1	2.18	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:N	1:A:323:MET:SD	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:264:VAL:O	1:A:265:THR:C	2.40	0.60
1:A:77:LEU:O	1:A:80:ILE:HB	2.01	0.60
1:B:307:SER:HA	1:B:379:GLN:HE21	1.66	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:A:40:ILE:HD13	1:A:45:THR:HG22	1.83	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:279:ALA:O	1:B:283:ILE:HG12	2.01	0.60
1:B:95:PHE:O	1:B:96:GLY:C	2.40	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:338:THR:CG2	1:B:339:SER:N	2.64	0.59
1:B:66:LEU:O	1:B:70:LEU:HG	2.01	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:239:PHE:C	1:B:239:PHE:CD1	2.75	0.59
1:B:9:PHE:HD2	1:B:10:TRP:HE3	1.49	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: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:B:224:PHE:CD2	1:B:399:THR:CG2	2.86	0.59
1:B:50:ALA:O	1:B:53:SER:HB3	2.03	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:158:VAL:O	1:B:162:PHE:N	2.30	0.58
1:B:85:VAL:HG13	1:B:178:LEU:HB2	1.85	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: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: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:A:90:PHE:CE2	1:A:95:PHE:HE1	2.20	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:348:THR:HA	1:A:351:LEU:HD12	1.85	0.58
1:A:4:LEU:HD22	1:A:10:TRP:CZ3	2.37	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:121:GLY:CA	1:B:124:ALA:HB3	2.34	0.58
1:B:20:PHE:H	1:B:20:PHE:HD1	1.52	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:154:GLY:O	1:A:155:ALA:C	2.43	0.57
1:A:10:TRP:CZ2	1:B:168:PHE:CE1	2.92	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:148:CYS:O	1:B:148:CYS:SG	2.63	0.57
1:B:278:PHE:CD1	1:B:278:PHE:N	2.73	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: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:A:74:LYS:H	1:A:74:LYS:CD	2.15	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:113:TYR:C	1:A:115:GLY:N	2.55	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: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:H	1:B:263:TYR:HD1	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:C	1:A:239:PHE:CD1	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:90:PHE:CB	1:A:114:LEU:HD13	2.36	0.56
1:A:198:ALA:HB3	1:A:201:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD11	1:A:162:PHE:HZ	1.65	0.56
1:B:48:ILE:HA	1:B:108:ILE:CG2	2.32	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CD2	2.24	0.56
1:B:278:PHE:HD1	1:B:278:PHE:N	2.03	0.56
1:A:108:ILE:O	1:A:112:ILE:HG13	2.05	0.56
1:A:2:TYR:CE1	1:A:137:ASN:ND2	2.74	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:HD1	1:B:239:PHE:C	2.09	0.55
1:A:12:PHE:O	1:A:15:PHE:N	2.39	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:A:44:ASP:HA	1:A:104:LEU:CD2	2.36	0.55
1:B:116:PHE:C	1:B:118:PHE:H	2.10	0.55
1:B:85:VAL:CG2	1:B:178:LEU:HD13	2.36	0.55
1:B:50:ALA:HB1	1:B:363:ILE:HA	1.89	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:215:GLU:C	1:A:215:GLU:OE1	2.45	0.55
1:A:24:GLY:O	1:A:25:ALA: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:85:VAL:CG2	1:A:178:LEU:HD13	2.35	0.55
1:A:17:PHE:HD2	1:A:18:PHE:CE2	2.25	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:279:ALA:O	1:B:282:ILE:HB	2.07	0.55
1:B:44:ASP:HA	1:B:104:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:O	1:B:48:ILE:C	2.42	0.55
1:A:121:GLY:HA2	1:A:124:ALA:CB	2.34	0.54
1:A:29:PHE:HE1	1:A:33:TRP:CD1	2.25	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:311:SER:O	1:A:314:GLU:HB3	2.07	0.54
1:A:55:PHE:O	1:A:59:PHE:HB2	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:246:PHE:HD1	1:B:246:PHE:C	2.09	0.54
1:B:33:TRP:CD1	1:B:37:ILE:HD13	2.43	0.54
1:A:13:GLY:O	1:A:146:PHE:HD2	1.91	0.54
1:B:42:LYS:HZ2	1:B:373:TYR:HB3	1.73	0.54
1:B:40:ILE:HD13	1:B:45:THR:HG22	1.90	0.54
1:A:55:PHE:CZ	1:A:113:TYR:HE1	2.27	0.53
1:A:307:SER:C	1:A:379:GLN:NE2	2.61	0.53
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.90	0.53
1:A:10:TRP:NE1	1:B:168:PHE:HD1	2.03	0.53
1:B:24:GLY:O	1:B:25:ALA:C	2.44	0.53
1:A:239:PHE:C	1:A:239:PHE:HD1	2.12	0.53
1:A:47:ILE:O	1:A:48:ILE:C	2.47	0.53
1:B:125:VAL:O	1:B:129:ILE:HG13	2.08	0.53
1:B:20:PHE:HB3	1:B:151:TRP:CA	2.38	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:OE1	1:B:215:GLU:C	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:174:SER:O	1:A:177:ALA:HB3	2.09	0.53
1:A:90:PHE:O	1:A:94:ILE:HG13	2.09	0.53
1:B:112:ILE:O	1:B:112:ILE:HG22	2.09	0.53
1:B:1:MET:O	1:B:2:TYR:C	2.47	0.53
1:B:319:LYS:O	1:B:322:HIS:N	2.31	0.53
1:B:42:LYS:NZ	1:B:378:PHE:CE1	2.77	0.53
1:A:85:VAL:CG2	1:A:178:LEU:HB2	2.38	0.53
1:A:17:PHE:HD2	1:A:18:PHE:CD2	2.27	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: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:A:95:PHE:O	1:A:96:GLY:C	2.46	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:HD3	1:A:135:ARG:O	2.10	0.52
1:B:224:PHE:N	1:B:224:PHE:CD1	2.76	0.52
1:B:239:PHE:HE2	1:B:303:ILE:HA	1.73	0.52
1:A:112:ILE:O	1:A:112:ILE:HG22	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:HD1	1:A:246:PHE:C	2.13	0.52
1:B:12:PHE:O	1:B:15:PHE:N	2.42	0.52
1:B:151:TRP:HD1	1:B:269:GLU:HG3	1.73	0.52
1:B:373:TYR:HE1	1:B:382:TYR:HE1	1.58	0.52
1:B:303:ILE:HG21	1:B:386:GLY:CA	2.39	0.52
1:B:78:TRP:C	1:B:80:ILE:N	2.63	0.52
1:B:77:LEU:O	1:B:80:ILE:HB	2.10	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:N	1:A:278:PHE:HD1	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:336:TYR:OH	1:B:401:SER:HB2	2.10	0.52
1:B:289:LYS:HD2	1:B:401:SER:O	2.10	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: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:B:62:LEU:O	1:B:62:LEU:HD12	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:136:SER:O	1:A:137:ASN:HB2	2.10	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:B:239:PHE:CE2	1:B:303:ILE:HG12	2.45	0.51
1:A:127:ALA:O	1:A:130:GLU:HB3	2.11	0.51
1:A:18:PHE:CZ	1:A:180:LEU:CD1	2.94	0.51
1:A:1:MET:SD	1:A:3:TYR:OH	2.58	0.51
1:A:70:LEU:HD11	1:A:76:LEU:HB2	1.92	0.51
1:A:9:PHE:CD2	1:A:10:TRP:CE3	2.98	0.51
1:B:226:SER:O	1:B:227:LEU:C	2.49	0.51
1:B:34:LEU:HD13	1:B:40:ILE:CD1	2.36	0.51
1:A:178:LEU:HG	1:A:179:ILE:N	2.26	0.51
1:A:135:ARG:NH2	1:A:192:PRO:HA	2.26	0.51
1:A:33:TRP:HH2	1:A:95:PHE:HB2	1.76	0.51
1:B:40:ILE:HG13	1:B:44:ASP:HB2	1.92	0.51
1:B:8:ASN:ND2	1:B:189:THR:OG1	2.44	0.51
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:A:33:TRP:CD1	1:A:37:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:290:ASN:O	1:A:291:ALA:C	2.48	0.51
1:A:225:LEU:HD13	1:A:336:TYR:HE2	1.76	0.51
1:A:390:LEU:HD23	1:A:390:LEU:C	2.32	0.51
1:A:224:PHE:CD2	1:A:399:THR:CG2	2.94	0.51
1:A:78:TRP:O	1:A:80:ILE:N	2.43	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: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:315:VAL:O	1:A:316:VAL:C	2.49	0.50
1:A:236:TYR:HH	1:A:322:HIS:HD1	1.56	0.50
1:A:40:ILE:HG13	1:A:44:ASP:HB2	1.93	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: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:29:PHE:CE1	1:B:170:PHE:CZ	3.00	0.50
1:B:303:ILE:O	1:B:306:SER:N	2.41	0.50
1:A:244:ALA:O	1:A:245:ASN:C	2.50	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: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:336:TYR:CE2	1:A:400:LEU:HD11	2.47	0.49
1:A:9:PHE:O	1:A:10:TRP:C	2.50	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:116:PHE:CD1	1:B:116:PHE:C	2.85	0.49
1:B:400:LEU:HG	1:B:401:SER:N	2.27	0.49
1:B:55:PHE:CZ	1:B:113:TYR:HE1	2.30	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:90:PHE:CB	1:B:114:LEU:HD13	2.41	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: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:161:MET:HB3	1:A:168:PHE:HE2	1.78	0.49
1:A:25:ALA:O	1:A:26:TYR:C	2.50	0.49
1:B:101:TYR:O	1:B:102:ASN:HB2	2.13	0.49
1:B:99:LEU:HD23	1:B:104:LEU:HA	1.95	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:289:LYS:O	1:B:293:LEU:HG	2.13	0.49
1:B:51:ALA:O	1:B:54:LEU:N	2.46	0.49
1:B:246:PHE:HB2	1:B:378:PHE:HD2	1.70	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:A:99:LEU:HG	1:A:107:SER:OG	2.12	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: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:366:SER:O	1:A:369:ALA:HB3	2.13	0.48
1:A:336:TYR:CZ	1:A:400:LEU:HD11	2.48	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: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:CD1	1:A:93:PHE:N	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:55:PHE:CZ	1:A:113:TYR:CE1	3.02	0.48
1:A:1:MET:HA	1:A:5:LYS:HE3	1.96	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:128:PHE:CD1	1:B:128:PHE:C	2.85	0.48
1:B:25:ALA:O	1:B:26:TYR:C	2.52	0.48
1:B:40:ILE:HG12	1:B:41:SER:O	2.14	0.48
1:B:33:TRP:HH2	1:B:95:PHE:HB2	1.79	0.48
1:A:228:TYR:O	1:A:229:VAL:C	2.53	0.47
1:A:90:PHE:HD1	1:A:94:ILE:HD12	1.68	0.47
1:B:136:SER:O	1:B:137:ASN:HB3	2.13	0.47
1:B:78:TRP:C	1:B:80:ILE:H	2.17	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:B:178:LEU:HG	1:B:179:ILE:N	2.30	0.47
1:B:1:MET:HA	1:B:5:LYS:HE3	1.97	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:52:ILE:HG12	1:B:112:ILE:HG23	1.95	0.47
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:38:ASN:HA	1:B:100:GLN:NE2	2.30	0.47
1:B:114:LEU:O	1:B:114:LEU:HD23	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:91:PHE:HB3	1:B:170:PHE:CE2	2.49	0.47
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.50	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:93:PHE:N	1:B:93:PHE:CD1	2.82	0.47
1:A:223:TRP:CE3	1:A:223:TRP:HA	2.50	0.47
1:A:303:ILE:O	1:A:306:SER:N	2.39	0.47
1:A:212:LEU:HD22	1:A:345:PHE:CE1	2.49	0.47
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.97	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:332:GLY:O	1:B:333:CYS:C	2.53	0.47
1:B:45:THR:OG1	1:B:46:GLY:N	2.47	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:HE3	1:B:223:TRP:HA	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:345:PHE:O	1:A:346:SER:C	2.54	0.46
1:A:90:PHE:CZ	1:A:95:PHE:HE1	2.34	0.46
1:A:9:PHE:HE2	1:A:10:TRP:CZ3	2.34	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:175:GLY:O	1:B:176:CYS:C	2.54	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:A:57:LEU:HD13	1:A:355:CYS:O	2.16	0.46
1:B:100:GLN:C	1:B:102:ASN:H	2.17	0.46
1:B:32:ILE:HD13	1:B:258:THR:HG23	1.97	0.46
1:B:320:THR:C	1:B:322:HIS:N	2.69	0.46
1:A:157:ILE:CG2	1:A:161:MET:HG3	2.45	0.46
1:A:223:TRP:HE3	1:A:223:TRP:HA	1.81	0.46
1:A:40:ILE:HG12	1:A:41:SER:O	2.16	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:139:GLU:C	1:A:141:GLY:N	2.69	0.46
1:A:17:PHE:CD2	1:A:18:PHE:CE2	3.03	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:135:ARG:HH21	1:A:192:PRO:CA	2.29	0.45
1:A:51:ALA:O	1:A:52:ILE:C	2.55	0.45
1:B:107:SER:O	1:B:111:GLY:HA3	2.16	0.45
1:B:27:PHE:HB3	1:B:28:PRO:HD3	1.94	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:227:LEU:HA	1:A:227:LEU:HD23	1.88	0.45
1:A:30:PHE:O	1:A:31:PRO:C	2.51	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:224:PHE:N	1:B:224:PHE:HD1	2.13	0.45
1:B:259:ARG:O	1:B:262:GLY:N	2.50	0.45
1:B:228:TYR:OH	1:B:292:LEU:O	2.33	0.45
1:B:72:LEU:O	1:B:72:LEU:HG	2.17	0.45
1:A:208:PHE:CD2	1:A:351:LEU:HD13	2.52	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: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:116:PHE:C	1:A:116:PHE:CD1	2.88	0.45
1:A:12:PHE:C	1:A:14:LEU:N	2.69	0.45
1:A:175:GLY:O	1:A:176:CYS:C	2.55	0.45
1:A:42:LYS:O	1:A:43:SER: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:HE2	1:A:11:MET:HA	1.99	0.45
1:B:30:PHE:O	1:B:31:PRO:C	2.55	0.45
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: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:B:327:PRO:HG2	1:B:328:PHE:H	1.82	0.44
1:B:33:TRP:HH2	1:B:95:PHE:CB	2.30	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: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:N	1:B:263:TYR:HD1	2.15	0.44
1:B:42:LYS:HB2	1:B:374:GLU:HB2	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:246:PHE:CD1	1:A:247:PHE:N	2.83	0.44
1:B:217:PHE:HD2	1:B:223:TRP:HH2	1.65	0.44
1:B:345:PHE:O	1:B:346:SER:C	2.55	0.44
1:B:307:SER:O	1:B:379:GLN:NE2	2.50	0.44
1:B:97:PRO:O	1:B:98:LEU:C	2.52	0.44
1:A:307:SER:HA	1:A:379:GLN:HB3	1.99	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:B:40:ILE:CG1	1:B:44:ASP:HB2	2.48	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: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:B:51:ALA:O	1:B:52:ILE:C	2.55	0.44
1:A:250:PHE:CD1	1:A:250:PHE:N	2.86	0.44
1:B:329:LEU:HA	1:B:329:LEU:HD12	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:CD1	1:A:382:TYR:N	2.86	0.43
1:B:139:GLU:C	1:B:141:GLY:N	2.71	0.43
1:B:40:ILE:CD1	1:B:48:ILE:HD12	2.47	0.43
1:A:113:TYR:C	1:A:115:GLY:H	2.20	0.43
1:A:85:VAL:CG1	1:A:178:LEU:HD22	2.48	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:135:ARG:NH2	1:A:192:PRO:C	2.72	0.43
1:A:40:ILE:CD1	1:A:48:ILE:HD12	2.49	0.43
1:B:134:ARG:NH1	1:B:203:ALA:CA	2.80	0.43
1:B:13:GLY:O	1:B:146:PHE:CD2	2.70	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: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:A:55:PHE:CE1	1:A:113:TYR:CE1	3.07	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:B:50:ALA:O	1:B:51:ALA:C	2.57	0.43
1:A:53:SER:O	1:A:56:SER:N	2.48	0.43
1:B:320:THR:C	1:B:322:HIS:H	2.22	0.43
1:B:57:LEU:HD13	1:B:355:CYS:O	2.19	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:299:MET:O	1:B:302:ARG:N	2.52	0.43
1:B:78:TRP:NE1	1:B:185:PHE:CD1	2.87	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:100:GLN:C	1:B:102:ASN:N	2.72	0.43
1:B:23:MET:O	1:B:26:TYR:HB3	2.19	0.43
1:B:346:SER:O	1:B:347:ALA:C	2.57	0.43
1:B:78:TRP:O	1:B:80:ILE:N	2.51	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:26:TYR:O	1:A:27:PHE:C	2.58	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: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:A:2:TYR:CE2	1:A:3:TYR:CD2	3.07	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:B:9:PHE:HE2	1:B:10:TRP:CZ3	2.36	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:288:GLY:O	1:A:291:ALA:N	2.52	0.42
1:A:264:VAL:CG1	1:A:319:LYS:HG2	2.33	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:154:GLY:O	1:A:157:ILE:N	2.52	0.42
1:A:37:ILE:CD1	1:A:162:PHE:HZ	2.32	0.42
1:A:91:PHE:CD2	1:A:170:PHE:CZ	3.07	0.42
1:A:372:MET:O	1:A:376:ILE:HB	2.20	0.42
1:A:85:VAL:O	1:A:174:SER:OG	2.36	0.42
1:B:369:ALA:O	1:B:370:GLY:C	2.57	0.42
1:B:2:TYR:CE2	1:B:3:TYR:CD2	3.07	0.42
1:A:25:ALA:O	1:A:29:PHE:CB	2.67	0.42
1:A:53:SER:OG	1:A:363:ILE:HG13	2.20	0.42
1:A:42:LYS:HB2	1:A:374:GLU:HB2	2.00	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:299:MET:O	1:B:303:ILE:HG13	2.20	0.42
1:B:293:LEU:HD22	1:B:397:VAL:CG2	2.50	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: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: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:373:TYR:O	1:B:377:GLY:N	2.44	0.42
1:B:54:LEU:HA	1:B:363:ILE:HD11	2.01	0.42
1:B:9:PHE:O	1:B:10:TRP:C	2.58	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:26:TYR:O	1:B:27:PHE:C	2.58	0.42
1:B:8:ASN:O	1:B:9:PHE:C	2.55	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:HG13	1:B:22:ILE:H	1.64	0.42
1:B:373:TYR:CE1	1:B:382:TYR:HE1	2.36	0.42
1:B:40:ILE:HD11	1:B:45:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:72:LEU:O	1:A:72:LEU:HG	2.20	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:264:VAL:CG1	1:B:319:LYS:HG2	2.37	0.41
1:B:60:GLN:HG2	1:B:60:GLN:O	2.19	0.41
1:A:10:TRP:HB3	1:A:11:MET:CE	2.49	0.41
1:A:299:MET:SD	1:A:325:GLU:OE2	2.78	0.41
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.50	0.41
1:A:327:PRO:HG2	1:A:328:PHE:H	1.84	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.87	0.41
1:A:8:ASN:O	1:A:9:PHE:C	2.56	0.41
1:B:135:ARG:HH21	1:B:192:PRO:CA	2.33	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: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:SG	1:A:148:CYS:O	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: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:33:TRP:CE3	1:B:38:ASN:ND2	2.89	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:178:LEU:O	1:A:179:ILE:C	2.59	0.41
1:A:51:ALA:O	1:A:54:LEU:N	2.54	0.41
1:B:137:ASN:O	1:B:137:ASN:OD1	2.38	0.41
1:A:337:ILE:O	1:A:341:PHE:HB2	2.21	0.41
1:A:40:ILE:HD11	1:A:45:THR:N	2.36	0.41
1:A:62:LEU:C	1:A:62:LEU:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HH2	1:A:95:PHE:CB	2.34	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:B:62:LEU:C	1:B:62:LEU:HD12	2.41	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:38:ASN:HA	1:A:100:GLN:NE2	2.36	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: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:A:14:LEU:O	1:A:15:PHE:C	2.60	0.41
1:A:22:ILE:HG13	1:A:22:ILE:H	1.59	0.41
1:A:248:THR:HG22	1:A:248:THR:O	2.21	0.41
1:A:277:PHE:HB3	1:A:278:PHE:CD1	2.55	0.41
1:A:250:PHE:HD2	1:A:311:SER:C	2.23	0.41
1:A:86:MET:O	1:A:90:PHE:CB	2.69	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:B:75:TYR:CE2	1:B:79:ILE:HD11	2.56	0.41
1:A:52:ILE:HA	1:A:112:ILE:HD13	2.03	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: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:N	1:A:20:PHE:CD1	2.85	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:A:50:ALA:O	1:A:51:ALA:C	2.58	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:HG2	1:A:302:ARG:O	2.20	0.40
1:A:337:ILE:O	1:A:338:THR:C	2.59	0.40
1:B:276:MET:C	1:B:278:PHE:N	2.75	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: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: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:A:10:TRP:CZ2	1:B:168:PHE:CD1	3.10	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
1:B:34:LEU:HD22	1:B:40:ILE:HD12	2.04	0.40







There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/417 (100%)	274 (66%)	102 (25%)	39 (9%)		
1	B	415/417 (100%)	271 (65%)	107 (26%)	37 (9%)		
All	All	830/834 (100%)	545 (66%)	209 (25%)	76 (9%)		

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 ⓘ

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%)	14	48
1	B	345/345 (100%)	317 (92%)	28 (8%)	14	48
All	All	690/690 (100%)	634 (92%)	56 (8%)	14	48

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

Some 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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.