



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

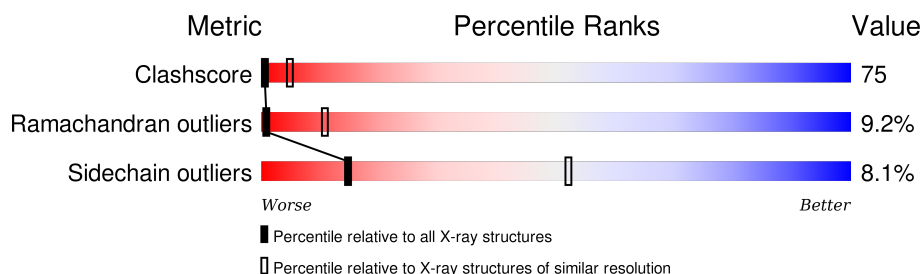
1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (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:

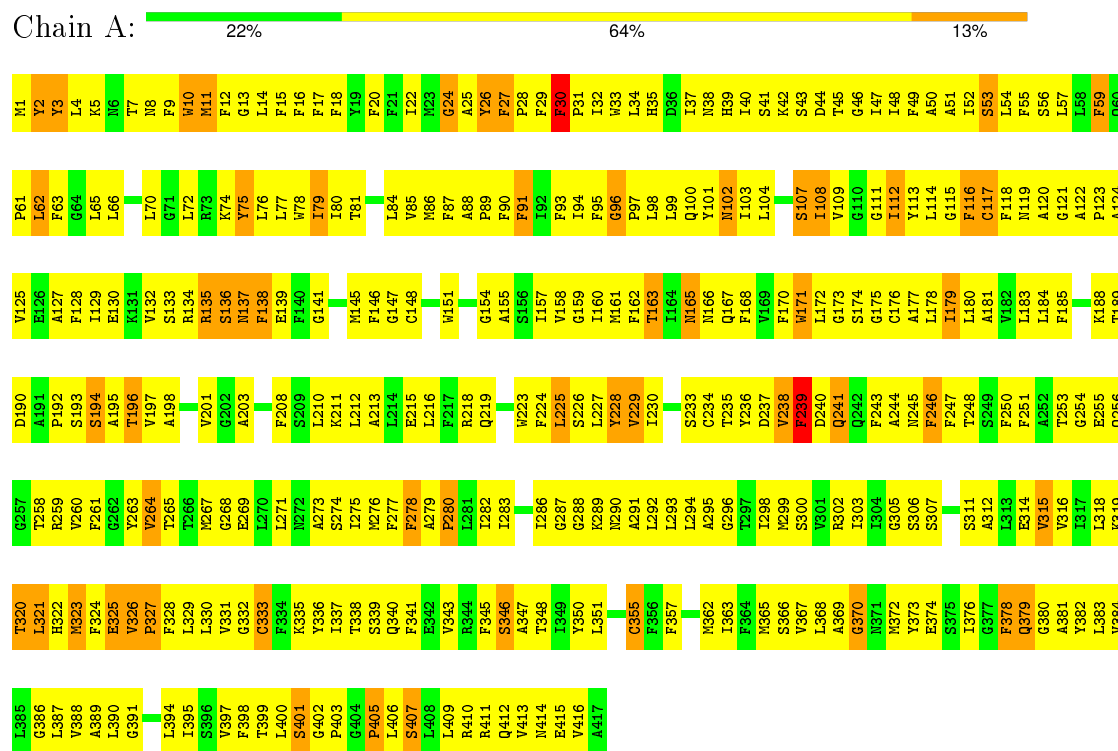
Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	ENGINEERED	UNP P02920
B	154	GLY	CYS	ENGINEERED	UNP P02920

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

Note EDS was not executed.

- Molecule 1: Lactose permease



- Molecule 1: Lactose permease



I385	I386	I388	I390	I391	I392	I393	I394	I395	I396	I397	I398	I399	I400	I401	I402	I403	I404	I405	I406	I407	I408	I409	I410	I411	I412	I413	I414	I415	I416	I417
G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426
E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355
V260	V261	V262	V263	V264	V265	V266	V267	V268	V269	V270	V271	V272	V273	V274	V275	V276	V277	V278	V279	V280	V281	V282	V283	V284	V285	V286	V287	V288	V289	V290
S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223
P192	P193	P194	P195	P196	P197	P198	P199	P200	P201	P202	P203	P204	P205	P206	P207	P208	P209	P210	P211	P212	P213	P214	P215	P216	P217	P218	P219	P220	P221	P222
A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221
T258	T259	T260	T261	T262	T263	T264	T265	T266	T267	T268	T269	T270	T271	T272	T273	T274	T275	T276	T277	T278	T279	T280	T281	T282	T283	T284	T285	T286	T287	T288
R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319
F261	F262	F263	F264	F265	F266	F267	F268	F269	F270	F271	F272	F273	F274	F275	F276	F277	F278	F279	F280	F281	F282	F283	F284	F285	F286	F287	F288	F289	F290	F291
S233	S234	S235	S236	S237	S238	S239	S240	S241	S242	S243	S244	S245	S246	S247	S248	S249	S250	S251	S252	S253	S254	S255	S256	S257	S258	S259	S260	S261	S262	S263
D223	D224	D225	D226	D227	D228	D229	D230	D231	D232	D233	D234	D235	D236	D237	D238	D239	D240	D241	D242	D243	D244	D245	D246	D247	D248	D249	D250	D251	D252	D253
Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249
W223	W224	W225	W226	W227	W228	W229	W230	W231	W232	W233	W234	W235	W236	W237	W238	W239	W240	W241	W242	W243	W244	W245	W246	W247	W248	W249	W250	W251	W252	W253
E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245
L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240
K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241
M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221	M222	M223	M224	M225	M226	M227	M228	M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241
N211	N212	N213	N214	N215	N216	N217	N218	N219	N220	N221	N222	N223	N224	N225	N226	N227	N228	N229	N230	N231	N232	N233	N234	N235	N236	N237	N238	N239	N240	N241
O211	O212	O213	O214	O215	O216	O217	O218	O219	O220	O221	O222	O223	O224	O225	O226	O227	O228	O229	O230	O231	O232	O233	O234	O235	O236	O237	O238	O239	O240	O241
P211	P212	P213	P214	P215	P216	P217	P218	P219	P220	P221	P222	P223	P224	P225	P226	P227	P228	P229	P230	P231	P232	P233	P234	P235	P236	P237	P238	P239	P240	P241
Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241
R211	R212	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241
S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223	S224	S225	S226	S227	S228	S229	S230	S231	S232	S233	S234	S235	S236	S237	S238	S239	S240	S241
T211	T212	T213	T214	T215	T216	T217	T218	T219	T220	T221	T222	T223	T224	T225	T226	T227	T228	T229	T230	T231	T232	T233	T234	T235	T236	T237	T238	T239	T240	T241
U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241
V211	V212	V213	V214	V215	V216	V217	V218	V219	V220	V221	V222	V223	V224	V225	V226	V227	V228	V229	V230	V231	V232	V233	V234	V235	V236	V237	V238	V239	V240	V241
W211	W212	W213	W214	W215	W216	W217	W218	W219	W220	W221	W222	W223	W224	W225	W226	W227	W228	W229	W230	W231	W232	W233	W234	W235	W236	W237	W238	W239	W240	W241
X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225	X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241
Y211	Y212	Y213	Y214	Y215	Y216	Y217	Y218	Y219	Y220	Y221	Y222	Y223	Y224	Y225	Y226	Y227	Y228	Y229	Y230	Y231	Y232	Y233	Y234	Y235	Y236	Y237	Y238	Y239	Y240	Y241
Z211	Z212	Z213	Z214	Z215	Z216	Z217	Z218	Z219	Z220	Z221	Z222	Z223	Z224	Z225	Z226	Z227	Z228	Z229	Z230	Z231	Z232	Z233	Z234	Z235	Z236	Z237	Z238	Z239	Z240	Z241
A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221
B191	B192	B193	B194	B195	B196	B197	B198	B199	B200	B201	B202	B203	B204	B205	B206	B207	B208	B209	B210	B211	B212	B213	B214	B215	B216	B217	B218	B219	B220	B221
C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221
D191	D192	D193	D194	D195	D196	D197	D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	D211	D212	D213	D214	D215	D216	D217	D218	D219	D220	D221
E191	E192	E193	E194	E195	E196	E197	E198	E199	E200	E201	E202	E203	E204	E205	E206	E207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221
F191	F192	F193	F194	F195	F196	F197	F198	F199	F200	F201	F202	F203	F204	F205	F206	F207	F208	F209	F210	F211	F212	F213	F214	F215	F216	F217	F218	F219	F220	F221
G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221
H191	H192	H193	H194	H195	H196	H197	H198	H199	H200	H201	H202	H203	H204	H205	H206	H207	H208	H209	H210	H211	H212	H213	H214	H215	H216	H217	H218	H219	H220	H221
I191	I192	I193	I194	I195	I196	I197	I198	I199	I200	I201	I202	I203	I204	I205	I206	I207	I208	I209	I210	I211	I212	I213	I214	I215	I216	I217	I218	I219	I220	I221
J191	J192	J193	J194	J195	J196	J197	J198	J199	J200	J201	J202	J203	J204	J205	J206	J207	J208	J209	J210	J211	J212	J213	J214	J215	J216	J217	J218	J219	J220	J221
K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221
L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221
M191	M192	M193	M194	M195	M196	M197	M198	M199	M200	M201	M202	M203	M204	M205	M206	M207	M208	M209	M210	M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221
N191	N192	N193	N194	N195	N196	N197	N198	N199	N200	N201	N202	N203	N204	N205	N206	N207	N208	N209	N210	N211	N212	N213	N214	N215	N216	N217	N218	N219	N220	N221
O191	O192	O193	O194	O195	O196	O197	O198	O199	O200	O201	O202	O203	O204	O205	O206	O207	O208	O209	O210	O211	O212	O213	O214	O215	O216	O217	O218	O219	O220	O221
P191	P192	P193	P194	P195	P196	P197	P198	P199	P200	P201	P202	P203	P204	P205	P206	P207	P208	P209	P210	P211	P212	P213	P214	P215	P216	P217	P218	P219	P220	P221
Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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:B:264:VAL:HG11	1:B:319:LYS:HG2	1.51	0.92
1:A:77:LEU:HD12	1:A:80:ILE:HD12	1.50	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:B:34:LEU:HD13	1:B:40:ILE:HD13	1.58	0.85
1:A:256:GLN:OE1	1:A:259:ARG:HD2	1.75	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:B:289:LYS:HE3	1:B:400:LEU:HB3	1.62	0.82
1:A:85:VAL:HG21	1:A:178:LEU:HD13	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:B:37:ILE:HD13	1:B:166:ASN:HD22	1.48	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:A:121:GLY:HA2	1:A:124:ALA:HB3	1.65	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:N	1:A:74:LYS:HD2	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: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:B:16:PHE:HB3	1:B:147:GLY:HA3	1.69	0.75
1:B:33:TRP:O	1:B:37:ILE:HB	1.85	0.75
1:A:16:PHE:HB3	1:A:147:GLY:HA3	1.69	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:B:27:PHE:HB3	1:B:28:PRO:HD2	1.68	0.74
1:B:99:LEU:CD2	1:B:104:LEU:HD12	2.16	0.74
1:A:1:MET:HB2	1:A:3:TYR:CZ	2.23	0.74
1:B:87:PHE:HB3	1:B:174:SER:HB2	1.69	0.74
1:B:271:LEU:HD23	1:B:323:MET:HB2	1.69	0.74
1:A:121:GLY:O	1:A:124:ALA:HB3	1.86	0.74
1:A:41:SER:O	1:A:45:THR:HG23	1.87	0.74
1:A:168:PHE:O	1:A:171:TRP:HB2	1.88	0.73
1:B:61:PRO:O	1:B:65:LEU:HG	1.88	0.73
1:B:246:PHE:CD1	1:B:246:PHE:C	2.62	0.73
1:A:44:ASP:HA	1:A:104:LEU:HD21	1.71	0.73
1:A:122:ALA:HB3	1:A:123:PRO:CD	2.18	0.73
1:B:1:MET:HB2	1:B:3:TYR:CZ	2.23	0.73
1:A:10:TRP:HZ2	1:B:168:PHE:CE1	2.07	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:93:PHE:O	1:B:97:PRO:HG2	1.90	0.72
1:B:171:TRP:CE3	1:B:171:TRP:HA	2.24	0.72
1:B:163:THR:HG21	1:B:255:GLU:HG3	1.71	0.72
1:B:121:GLY:HA2	1:B:124:ALA:HB3	1.71	0.72
1:A:340:GLN:HE22	1:A:405:PRO:HB3	1.54	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:27:PHE:HB3	1:A:28:PRO:HD2	1.71	0.72
1:A:122:ALA:HB3	1:A:123:PRO:HD2	1.71	0.72
1:B:335:LYS:O	1:B:338:THR:HG22	1.89	0.72
1:A: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:A:87:PHE:HB3	1:A:174:SER:HB2	1.71	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:338:THR:HG21	1:A:415:GLU:OE2	1.91	0.71
1:A:165:ASN:O	1:A:168:PHE:HB3	1.89	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:338:THR:HG21	1:B:415:GLU:OE2	1.92	0.69
1:B:216:LEU:HD23	1:B:219:GLN:OE1	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:90:PHE:CZ	1:A:114:LEU:HB3	2.28	0.69
1:B:119:ASN:O	1:B:123:PRO:HD2	1.93	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:90:PHE:CZ	1:B:114:LEU:HB3	2.28	0.69
1:A:74:LYS:HD2	1:A:74:LYS:H	1.53	0.69
1:A:66:LEU:O	1:A:70:LEU:HG	1.92	0.69
1:A:289:LYS:HA	1:A:400:LEU:HD21	1.74	0.68
1:A:22:ILE:HB	1:A:118:PHE:CZ	2.27	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:172:LEU:HD13	1:B:183:LEU:CD1	2.25	0.67
1:A:171:TRP:CE3	1:A:171:TRP:HA	2.29	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:246:PHE:HB2	1:A:378:PHE:CE2	2.30	0.66
1:A:216:LEU:HD23	1:A:219:GLN:OE1	1.95	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:B:50:ALA:HB2	1:B:366:SER:CB	2.24	0.65
1:A:4:LEU:HD22	1:A:10:TRP:HZ3	1.61	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:B:289:LYS:HA	1:B:400:LEU:HD21	1.77	0.65
1:A:271:LEU:HD23	1:A:323:MET:HB2	1.78	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:289:LYS:HD3	1:A:403:PRO:HG3	1.77	0.65
1:A:48:ILE:HA	1:A:108:ILE:CG2	2.27	0.65
1:B:323:MET:N	1:B:323:MET:SD	2.70	0.65
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.32	0.65
1:A:158:VAL:O	1:A:162:PHE:N	2.22	0.64
1:A:10:TRP:HB3	1:A:11:MET:HE3	1.80	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:B:90:PHE:CD2	1:B:114:LEU:HD22	2.32	0.64
1:A:121:GLY:CA	1:A:124:ALA:HB3	2.27	0.64
1:B:282:ILE:O	1:B:286:ILE:HG13	1.98	0.64
1:B:108:ILE:O	1:B:111:GLY:N	2.29	0.64
1:A:26:TYR:CD1	1:A:27:PHE:N	2.66	0.64
1:B:29:PHE:CE1	1:B:33:TRP:CD1	2.86	0.64
1:B:283:ILE:HG13	1:B:331:VAL:CG1	2.27	0.63
1:B:292:LEU:HD21	1:B:333:CYS:N	2.13	0.63
1:A:99:LEU:HD22	1:A:104:LEU:HD12	1.81	0.63
1:A:108:ILE:O	1:A:111:GLY:N	2.32	0.63
1:A:196:THR:HG21	1:A:201:VAL:CB	2.26	0.63
1:B:127:ALA:O	1:B:130:GLU:N	2.31	0.63
1:A:307:SER:HA	1:A:379:GLN:HE21	1.63	0.63
1:B:16:PHE:HB3	1:B:147:GLY:CA	2.29	0.63
1:B:161:MET:HB3	1:B:168:PHE:HE2	1.64	0.63
1:A:32:ILE:HD13	1:A:258:THR:HG23	1.79	0.63
1:A:34:LEU:HD13	1:A:40:ILE:CD1	2.24	0.63
1:A:279:ALA:O	1:A:283:ILE:HG12	1.98	0.62
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: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:A:133:SER:HG	1:A:138:PHE:C	2.02	0.62
1:B:76:LEU:HA	1:B:79:ILE:HD12	1.80	0.62
1:B:107:SER:O	1:B:111:GLY:N	2.32	0.62
1:A:239:PHE:CE2	1:A:303:ILE:HG12	2.34	0.62
1:B:90:PHE:CE2	1:B:95:PHE:HE1	2.18	0.62
1:B:323:MET:O	1:B:327:PRO:HD2	1.99	0.62
1:A:171:TRP:HA	1:A:171:TRP:HE3	1.65	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:B:379:GLN:O	1:B:382:TYR:HB2	1.99	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:161:MET:HB3	1:B:168:PHE:CE2	2.35	0.62
1:B:277:PHE:C	1:B:278:PHE:HD1	2.03	0.62
1:A:16:PHE:CE1	1:A:129:ILE:HD12	2.35	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:B:52:ILE:N	1:B:112:ILE:HD13	2.16	0.61
1:A:289:LYS:HG3	1:A:400:LEU:CD2	2.19	0.61
1:B:243:PHE:O	1:B:246:PHE:HB3	2.01	0.61
1:B:177:ALA:O	1:B:181:ALA:HB2	2.00	0.61
1:B:12:PHE:HE2	1:B:132:VAL:HG21	1.66	0.61
1:B:246:PHE:HD1	1:B:247:PHE:N	1.99	0.61
1:A:323:MET:N	1:A:323:MET:SD	2.73	0.61
1:B:289:LYS:HD3	1:B:403:PRO:HG3	1.81	0.61
1:B:44:ASP:OD1	1:B:104:LEU:HD22	2.01	0.61
1:B:368:LEU:O	1:B:372:MET:HG3	2.01	0.60
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: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:A:337:ILE:CD1	1:A:350:TYR:HE1	2.14	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:B:307:SER:HA	1:B:379:GLN:HE21	1.66	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:A:107:SER:O	1:A:111:GLY:N	2.35	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:A:277:PHE:C	1:A:278:PHE:HD1	2.05	0.60
1:A:283:ILE:HG13	1:A:331:VAL:HG11	1.82	0.60
1:B:9:PHE:CD2	1:B:10:TRP:HE3	2.20	0.60
1:B:165:ASN:O	1:B:168:PHE:HB3	2.02	0.60
1:B:49:PHE:HB3	1:B:241:GLN:OE1	2.01	0.60
1:B:95:PHE:O	1:B:96:GLY:C	2.40	0.60
1:B:279:ALA:O	1:B:283:ILE:HG12	2.01	0.60
1:A:20:PHE:HB3	1:A:151:TRP:HB2	1.83	0.59
1:A:340:GLN:NE2	1:A:405:PRO:HB3	2.17	0.59
1:A:368:LEU:O	1:A:372:MET:HG3	2.02	0.59
1:A:198:ALA:HB3	1:A:201:VAL:HG23	1.84	0.59
1:B: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:B:239:PHE:C	1:B:239:PHE:CD1	2.75	0.59
1:A:20:PHE:HD1	1:A:20:PHE:H	1.50	0.59
1:A:246:PHE:HD1	1:A:247:PHE:N	2.01	0.59
1:B:9:PHE:HD2	1:B:10:TRP:HE3	1.49	0.59
1: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:50:ALA:O	1:B:53:SER:HB3	2.03	0.59
1:B:224:PHE:CD2	1:B:399:THR:CG2	2.86	0.59
1:B:276:MET:HA	1:B:279:ALA:HB2	1.83	0.59
1:A:63:PHE:CE1	1:A:124:ALA:HB2	2.38	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:40:ILE:HG12	1:B:45:THR:HG23	1.85	0.58
1:B:90:PHE:O	1:B:94:ILE:HG13	2.02	0.58
1:B:196:THR:HG21	1:B:201:VAL:CB	2.30	0.58
1:B:253:THR:HG22	1:B:254:GLY:N	2.17	0.58
1:B:90:PHE:HD1	1:B:94:ILE:HD12	1.67	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:A:62:LEU:O	1:A:66:LEU:HG	2.03	0.58
1:B:264:VAL:O	1:B:265:THR:C	2.42	0.58
1:A:76:LEU:HA	1:A:79:ILE:HD12	1.84	0.58
1:A:4:LEU:HD22	1:A:10:TRP:CZ3	2.37	0.58
1:A:348:THR:HA	1:A:351:LEU:HD12	1.85	0.58
1:B:294:LEU:O	1:B:298:ILE:HG13	2.03	0.58
1:A:410:ARG:O	1:A:413:VAL:HB	2.04	0.58
1:A:289:LYS:HA	1:A:400:LEU:CD2	2.34	0.58
1:A:127:ALA:O	1:A:130:GLU:N	2.36	0.58
1:B:390:LEU:C	1:B:390:LEU:HD23	2.24	0.58
1:B:20:PHE:H	1:B:20:PHE:HD1	1.52	0.58
1:B:121:GLY:CA	1:B:124:ALA:HB3	2.34	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: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:B:307:SER:C	1:B:379:GLN:NE2	2.57	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:A:135:ARG:HH21	1:A:192:PRO:HA	1.69	0.58
1:B:26:TYR:CD2	1:B:27:PHE:N	2.72	0.57
1:B:37:ILE:HD11	1:B:162:PHE:HZ	1.67	0.57
1:A:50:ALA:HB1	1:A:363:ILE:HA	1.86	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:A:154:GLY:O	1:A:155:ALA:C	2.43	0.57
1:B:346:SER:OG	1:B:347:ALA:N	2.36	0.57
1:B:225:LEU:HD13	1:B:336:TYR:HE2	1.69	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:29:PHE:HE1	1:B:33:TRP:CD1	2.23	0.57
1:A:134:ARG:NH1	1:A:203:ALA:HA	2.18	0.57
1:B:148:CYS:O	1:B:148:CYS:SG	2.63	0.57
1:B:42:LYS:HG3	1:B:374:GLU:N	2.20	0.57
1:B:278:PHE:CD1	1:B:278:PHE:N	2.73	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:74:LYS:H	1:A:74:LYS:CD	2.15	0.57
1:A:133:SER:OG	1:A:139:GLU:HA	2.05	0.57
1:B:133:SER:OG	1:B:139:GLU:HA	2.05	0.57
1:A:263:TYR:HD1	1:A:263:TYR:H	1.53	0.57
1:B:337:ILE:CD1	1:B:350:TYR:HE1	2.18	0.57
1:A:121:GLY:C	1:A:124:ALA:HB3	2.26	0.56
1:A:78:TRP:C	1:A:80:ILE:N	2.58	0.56
1:A:49:PHE:O	1:A:52:ILE:HB	2.04	0.56
1:A:93:PHE:O	1:A:97:PRO:HG2	2.04	0.56
1:A:113:TYR:C	1:A:115:GLY:N	2.55	0.56
1:A:253:THR:HG22	1:A:254:GLY:N	2.21	0.56
1:A:18:PHE:CE1	1:A:180:LEU:HD12	2.41	0.56
1:B:326:VAL:HB	1:B:327:PRO:HD2	1.83	0.56
1:B:263:TYR:H	1:B:263:TYR:HD1	1.53	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:B:48:ILE:HA	1:B:108:ILE:CG2	2.32	0.56
1:A:90:PHE:CB	1:A:114:LEU:HD13	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD11	1:A:162:PHE:HZ	1.65	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CD2	2.24	0.56
1:A:198:ALA:HB3	1:A:201:VAL:CG2	2.36	0.56
1:B:278:PHE:HD1	1:B:278:PHE:N	2.03	0.56
1:B:44:ASP:O	1:B:48:ILE:HG13	2.06	0.56
1:A:108:ILE:O	1:A:112:ILE:HG13	2.05	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CE2	2.24	0.56
1:A:2:TYR:CE1	1:A:137:ASN:ND2	2.74	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:B:239:PHE:HD1	1:B:239:PHE:C	2.09	0.55
1:A:63:PHE:CE2	1:A:76:LEU:HD21	2.41	0.55
1:B:50:ALA:HB1	1:B:363:ILE:HA	1.89	0.55
1:A:44:ASP:HA	1:A:104:LEU:CD2	2.36	0.55
1:A:12:PHE:O	1:A:15:PHE:N	2.39	0.55
1:B:85:VAL:CG2	1:B:178:LEU:HD13	2.36	0.55
1:A:338:THR:HG23	1:A:339:SER:N	2.21	0.55
1:B:116:PHE:C	1:B:118:PHE:H	2.10	0.55
1:A:208:PHE:HA	1:A:212:LEU:HD12	1.88	0.55
1:A:12:PHE:HE2	1:A:132:VAL:HG21	1.72	0.55
1:B:271:LEU:HD23	1:B:323:MET:CB	2.35	0.55
1:A:85:VAL:HG21	1:A:178:LEU:CD1	2.34	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:278:PHE:O	1:A:282:ILE:HG13	2.06	0.55
1:B:289:LYS:HA	1:B:400:LEU:CD2	2.35	0.55
1:B:25:ALA:HA	1:B:158:VAL:HG21	1.89	0.55
1:A:24:GLY:O	1:A:25:ALA:C	2.45	0.55
1:A:215:GLU:C	1:A:215:GLU:OE1	2.45	0.55
1:B:18:PHE:CE1	1:B:180:LEU:HD12	2.41	0.55
1:A:296:GLY:HA2	1:A:299:MET:HE3	1.88	0.55
1:A:224:PHE:CD1	1:A:224:PHE:N	2.72	0.55
1:B:136:SER:O	1:B:137:ASN:HB2	2.06	0.55
1:A:17:PHE:HD2	1:A:18:PHE:CE2	2.25	0.55
1:A:85:VAL:CG2	1:A:178:LEU:HD13	2.35	0.55
1:B:44:ASP:HA	1:B:104:LEU:CD2	2.36	0.55
1:B:47:ILE:O	1:B:48:ILE:C	2.42	0.55
1:A:228:TYR:CZ	1:A:292:LEU:HB3	2.42	0.55
1:B:279:ALA:O	1:B:282:ILE:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:SER:OG	1:A:347:ALA:N	2.40	0.55
1:A:29:PHE:HE1	1:A:33:TRP:CD1	2.25	0.54
1:A:121:GLY:HA2	1:A:124:ALA:CB	2.34	0.54
1:B:27:PHE:CB	1:B:28:PRO:CD	2.83	0.54
1:B:236:TYR:HH	1:B:322:HIS:HD1	1.51	0.54
1:B:127:ALA:O	1:B:130:GLU:HB3	2.08	0.54
1:B:275:ILE:HG21	1:B:327:PRO:CG	2.35	0.54
1:A:20:PHE:HB3	1:A:151:TRP:CA	2.37	0.54
1:B:124:ALA:O	1:B:127:ALA:N	2.39	0.54
1:A:326:VAL:O	1:A:327:PRO:C	2.45	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:B:108:ILE:O	1:B:109:VAL:C	2.46	0.54
1:B:151:TRP:CD1	1:B:269:GLU:HG3	2.42	0.54
1:A:336:TYR:OH	1:A:401:SER:HB2	2.07	0.54
1:A:283:ILE:HG13	1:A:331:VAL:HG12	1.90	0.54
1:B:338:THR:HG23	1:B:339:SER:N	2.22	0.54
1:B:135:ARG:O	1:B:135:ARG:HD3	2.08	0.54
1:A:78:TRP:C	1:A:80:ILE:H	2.11	0.54
1:B:307:SER:CA	1:B:379:GLN:NE2	2.71	0.54
1:A:336:TYR:OH	1:A:401:SER:CB	2.56	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: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:13:GLY:O	1:A:146:PHE:HD2	1.91	0.54
1:B:24:GLY:O	1:B:25:ALA:C	2.44	0.53
1:A:307:SER:C	1:A:379:GLN:NE2	2.61	0.53
1:A:10:TRP:NE1	1:B:168:PHE:HD1	2.03	0.53
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.90	0.53
1:A:55:PHE:CZ	1:A:113:TYR:HE1	2.27	0.53
1:B:20:PHE:HB3	1:B:151:TRP:CA	2.38	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:275:ILE:CG2	1:B:327:PRO:HG3	2.35	0.53
1:B:113:TYR:O	1:B:116:PHE:HD2	1.91	0.53
1:B:215:GLU:OE1	1:B:215:GLU:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLY:O	1:B:145:MET:HG3	2.08	0.53
1:B:319:LYS:O	1:B:320:THR:C	2.46	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:28:PRO:O	1:B:29:PHE:C	2.46	0.53
1:A:307:SER:CA	1:A:379:GLN:NE2	2.71	0.53
1:A:278:PHE:N	1:A:278:PHE:CD1	2.77	0.53
1:B:49:PHE:O	1:B:52:ILE:HB	2.08	0.53
1:A:326:VAL:HB	1:A:327:PRO:HD2	1.87	0.53
1:A:277:PHE:HD2	1:A:278:PHE:CE1	2.27	0.53
1:B:33:TRP:HD1	1:B:37:ILE:HD13	1.74	0.53
1:B:112:ILE:O	1:B:112:ILE:HG22	2.09	0.53
1:B:319:LYS:O	1:B:322:HIS:N	2.31	0.53
1:B:42:LYS:NZ	1:B:378:PHE:CE1	2.77	0.53
1:A:90:PHE:O	1:A:94:ILE:HG13	2.09	0.53
1:B:1:MET:O	1:B:2:TYR:C	2.47	0.53
1:A:174:SER:O	1:A:177:ALA:HB3	2.09	0.53
1:A:244:ALA:O	1:A:247:PHE:N	2.42	0.53
1:A:17:PHE:HD2	1:A:18:PHE:CD2	2.27	0.53
1:B:277:PHE:HD2	1:B:278:PHE:CE1	2.27	0.53
1:A:85:VAL:CG2	1:A:178:LEU:HB2	2.38	0.53
1:B:299:MET:SD	1:B:325:GLU:OE2	2.66	0.52
1:A:289:LYS:O	1:A:293:LEU:HG	2.09	0.52
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.39	0.52
1:A:95:PHE:O	1:A:96:GLY:C	2.46	0.52
1:B:116:PHE:O	1:B:118:PHE:N	2.42	0.52
1:A:116:PHE:C	1:A:118:PHE:H	2.12	0.52
1:A:116:PHE:O	1:A:118:PHE:N	2.42	0.52
1:B:239:PHE:HE2	1:B:303:ILE:HA	1.73	0.52
1:B:224:PHE:N	1:B:224:PHE:CD1	2.76	0.52
1:A:135:ARG:HD3	1:A:135:ARG:O	2.10	0.52
1:A:112:ILE:O	1:A:112:ILE:HG22	2.10	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:A:107:SER:O	1:A:111:GLY:HA3	2.08	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:77:LEU:O	1:B:80:ILE:HB	2.10	0.52
1:B:78:TRP:C	1:B:80:ILE:N	2.63	0.52
1:A:226:SER:O	1:A:227:LEU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:MET:O	1:B:89:PRO:HD2	2.10	0.52
1:A:411:ARG:O	1:A:414:ASN:HB3	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:B:289:LYS:HD2	1:B:401:SER:O	2.10	0.52
1:B:336:TYR:OH	1:B:401:SER:HB2	2.10	0.52
1:A:382:TYR:O	1:A:383:LEU:C	2.46	0.52
1:A:289:LYS:HD2	1:A:401:SER:O	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: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:101:TYR:O	1:A:102:ASN:HB2	2.09	0.52
1:B:336:TYR:OH	1:B:401:SER:CB	2.58	0.51
1:A:289:LYS:CG	1:A:400:LEU:HD23	2.23	0.51
1:A:151:TRP:CD1	1:A:269:GLU:HG3	2.45	0.51
1:B:179:ILE:O	1:B:183:LEU:HB2	2.10	0.51
1:B:113:TYR:C	1:B:115:GLY:N	2.61	0.51
1:B:263:TYR:N	1:B:263:TYR:CD1	2.77	0.51
1:B:239:PHE:CE2	1:B:303:ILE:HG12	2.45	0.51
1:A:33:TRP:HD1	1:A:37:ILE:HD13	1.75	0.51
1:A:50:ALA:O	1:A:53:SER:HB3	2.10	0.51
1:A:136:SER:O	1:A:137:ASN:HB2	2.10	0.51
1:B:34:LEU:HD13	1:B:40:ILE:CD1	2.36	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:9:PHE:CD2	1:A:10:TRP:CE3	2.98	0.51
1:A:127:ALA:O	1:A:130:GLU:HB3	2.11	0.51
1:A:70:LEU:HD11	1:A:76:LEU:HB2	1.92	0.51
1:B:226:SER:O	1:B:227:LEU:C	2.49	0.51
1:A:178:LEU:HG	1:A:179:ILE:N	2.26	0.51
1:B:40:ILE:HG13	1:B:44:ASP:HB2	1.92	0.51
1:A:33:TRP:HH2	1:A:95:PHE:HB2	1.76	0.51
1:B:8:ASN:ND2	1:B:189:THR:OG1	2.44	0.51
1:A:135:ARG:NH2	1:A:192:PRO:HA	2.26	0.51
1:B:382:TYR:O	1:B:383:LEU:C	2.48	0.51
1:A:33:TRP:CD1	1:A:37:ILE:HD13	2.45	0.51
1:A:40:ILE:HG12	1:A:45:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:MET:HA	1:A:326:VAL:CG2	2.40	0.51
1:A:332:GLY:O	1:A:333:CYS:C	2.49	0.51
1:A:85:VAL:HG22	1:A:178:LEU:CB	2.39	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:225:LEU:HD13	1:A:336:TYR:HE2	1.76	0.51
1:A:290:ASN:O	1:A:291:ALA:C	2.48	0.51
1:A:1:MET:O	1:A:2:TYR:C	2.49	0.51
1:B:236:TYR:CG	1:B:299:MET:SD	3.04	0.51
1:A:78:TRP:O	1:A:80:ILE:N	2.43	0.51
1:A:224:PHE:CD2	1:A:399:THR:CG2	2.94	0.51
1:A:390:LEU:HD23	1:A:390:LEU:C	2.32	0.51
1:B:320:THR:O	1:B:322:HIS:N	2.44	0.50
1:A:34:LEU:CB	1:A:40:ILE:HG21	2.38	0.50
1:B:288:GLY:O	1:B:289:LYS:C	2.49	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:A:315:VAL:O	1:A:316:VAL:C	2.49	0.50
1:A:40:ILE:HG13	1:A:44:ASP:HB2	1.93	0.50
1:A:236:TYR:HH	1:A:322:HIS:HD1	1.56	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: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:B:289:LYS:HG3	1:B:400:LEU:CD2	2.23	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: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:173:GLY:O	1:A:177:ALA:HB2	2.12	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: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:A:336:TYR:CE2	1:A:400:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD22	1:B:10:TRP:CZ3	2.46	0.49
1:A:9:PHE:O	1:A:10:TRP:C	2.50	0.49
1:B:400:LEU:HG	1:B:401:SER:N	2.27	0.49
1:B:116:PHE:CD1	1:B:116:PHE:C	2.85	0.49
1:B:55:PHE:CZ	1:B:113:TYR:HE1	2.30	0.49
1:A:238:VAL:HA	1:A:241:GLN:NE2	2.27	0.49
1:A:121:GLY:O	1:A:125:VAL:N	2.43	0.49
1:A:161:MET:HB3	1:A:168:PHE:CE2	2.48	0.49
1:B:90:PHE:CB	1:B:114:LEU:HD13	2.41	0.49
1:B:86:MET:C	1:B:89:PRO:HD2	2.32	0.49
1:A:288:GLY:O	1:A:289:LYS:C	2.48	0.49
1:B:76:LEU:CD1	1:B:79:ILE:HD12	2.42	0.49
1:A:381:ALA:O	1:A:384:VAL:N	2.46	0.49
1:A:124:ALA:O	1:A:127:ALA:N	2.45	0.49
1:A:34:LEU:HD22	1:A:40:ILE:HD12	1.95	0.49
1:B:121:GLY:C	1:B:124:ALA:HB3	2.33	0.49
1:A:25:ALA:O	1:A:26:TYR:C	2.50	0.49
1:A:161:MET:HB3	1:A:168:PHE:HE2	1.78	0.49
1:B: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: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:A:224:PHE:N	1:A:224:PHE:HD1	2.09	0.49
1:B:246:PHE:HB2	1:B:378:PHE:HD2	1.70	0.48
1:B:29:PHE:CD1	1:B:33:TRP:HB2	2.48	0.48
1:A:99:LEU:HG	1:A:107:SER:OG	2.12	0.48
1:A:108:ILE:O	1:A:109:VAL:C	2.49	0.48
1:A:312:ALA:HA	1:A:315:VAL:HG23	1.95	0.48
1:B:407:SER:HG	1:B:410:ARG:HB2	1.79	0.48
1:A:157:ILE:HG23	1:A:161:MET:HG3	1.94	0.48
1:B:336:TYR:CZ	1:B:400:LEU:HD11	2.49	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:A:122:ALA:CB	1:A:123:PRO:CD	2.90	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: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:366:SER:O	1:A:369:ALA:HB3	2.13	0.48
1:A:97:PRO:O	1:A:98:LEU:C	2.52	0.48
1:A:320:THR:O	1:A:322:HIS:N	2.46	0.48
1:A:116:PHE:CG	1:A:117:CYS:N	2.81	0.48
1:A:84:LEU:HD21	1:A:117:CYS:HB3	1.95	0.48
1:B:62:LEU:O	1:B:66:LEU:HG	2.13	0.48
1:B:244:ALA:O	1:B:245:ASN:C	2.52	0.48
1:A:44:ASP:O	1:A:48:ILE:HG13	2.14	0.48
1:B:283:ILE:HG13	1:B:331:VAL:HG12	1.93	0.48
1:B:42:LYS:NZ	1:B:373:TYR:HB3	2.27	0.48
1:A:93:PHE:N	1:A:93:PHE:CD1	2.81	0.48
1:A:22:ILE:HD11	1:A:177:ALA:HB1	1.96	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: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:1:MET:HA	1:A:5:LYS:HE3	1.96	0.48
1:A:329:LEU:O	1:A:333:CYS:HB2	2.14	0.48
1:A:55:PHE:CZ	1:A:113:TYR:CE1	3.02	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:104:LEU:HG	1:A:108:ILE:HD11	1.95	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:A:213:ALA:O	1:A:216:LEU:N	2.47	0.48
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:228:TYR:O	1:A:229:VAL:C	2.53	0.47
1:A:362:MET:O	1:A:363:ILE:C	2.49	0.47
1:A:329:LEU:O	1:A:330:LEU:C	2.53	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: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:B:114:LEU:O	1:B:114:LEU:HD23	2.15	0.47
1:B:299:MET:O	1:B:300:SER:C	2.53	0.47
1:B:38:ASN:HA	1:B:100:GLN:NE2	2.30	0.47
1:B:1:MET:HA	1:B:5:LYS:HE3	1.97	0.47
1:A:8:ASN:ND2	1:A:189:THR:OG1	2.48	0.47
1:B:178:LEU:HG	1:B:179:ILE:N	2.30	0.47
1:B:271:LEU:HG	1:B:275:ILE:HD11	1.96	0.47
1:B:210:LEU:O	1:B:213:ALA:HB3	2.13	0.47
1:A:391:GLY:O	1:A:395:ILE:HG13	2.14	0.47
1:B:25:ALA:O	1:B:29:PHE:CB	2.62	0.47
1:B:91:PHE:HB3	1:B:170:PHE:CE2	2.49	0.47
1:B:93:PHE:N	1:B:93:PHE:CD1	2.82	0.47
1:A:16:PHE:HE1	1:A:129:ILE:CG2	2.24	0.47
1:B:70:LEU:HD11	1:B:76:LEU:HB2	1.96	0.47
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.50	0.47
1:A:400:LEU:HG	1:A:401:SER:N	2.30	0.47
1:A:303:ILE:O	1:A:306:SER:N	2.39	0.47
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.97	0.47
1:A:212:LEU:HD22	1:A:345:PHE:CE1	2.49	0.47
1:A:223:TRP:CE3	1:A:223:TRP:HA	2.50	0.47
1:B:45:THR:OG1	1:B:46:GLY:N	2.47	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: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:B:18:PHE:CZ	1:B:180:LEU:CD1	2.98	0.46
1:A:260:VAL:O	1:A:261:PHE:C	2.50	0.46
1:B:85:VAL:HG22	1:B:178:LEU:CB	2.43	0.46
1:B:247:PHE:HD2	1:B:315:VAL:CG1	2.27	0.46
1:A:315:VAL:O	1:A:318:LEU:N	2.47	0.46
1:A:123:PRO:O	1:A:127:ALA:HB2	2.15	0.46
1:B:154:GLY:O	1:B:155:ALA:C	2.54	0.46
1:A:394:LEU:O	1:A:397:VAL:HB	2.15	0.46
1:B:239:PHE:CD1	1:B:240:ASP:N	2.83	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:A:345:PHE:O	1:A:346:SER:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CZ	1:B:95:PHE:HE1	2.33	0.46
1:A:107:SER:O	1:A:111:GLY:CA	2.64	0.46
1:A:296:GLY:HA2	1:A:299:MET:CE	2.44	0.46
1:B:78:TRP:CD1	1:B:185:PHE:CE1	3.03	0.46
1:B:175:GLY:O	1:B:176:CYS:C	2.54	0.46
1:A:193:SER:O	1:A:194:SER:CB	2.64	0.46
1:B:100:GLN:C	1:B:102:ASN:H	2.17	0.46
1:B:320:THR:C	1:B:322:HIS:N	2.69	0.46
1:A:57:LEU:HD13	1:A:355:CYS:O	2.16	0.46
1:B:32:ILE:HD13	1:B:258:THR:HG23	1.97	0.46
1:B:382:TYR:N	1:B:382:TYR:CD1	2.83	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:A:157:ILE:CG2	1:A:161:MET:HG3	2.45	0.46
1:B:253:THR:CG2	1:B:254:GLY:N	2.79	0.46
1:A:223:TRP:HE3	1:A:223:TRP:HA	1.81	0.46
1:B:315:VAL:O	1:B:316:VAL:C	2.53	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: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:17:PHE:CD2	1:A:18:PHE:CE2	3.03	0.46
1:A:139:GLU:C	1:A:141:GLY:N	2.69	0.46
1:A:20:PHE:CE2	1:A:148:CYS:HA	2.51	0.46
1:B:122:ALA:CB	1:B:123:PRO:CD	2.92	0.46
1:A:271:LEU:O	1:A:275:ILE:HG13	2.16	0.46
1:A:51:ALA:O	1:A:52:ILE:C	2.55	0.45
1:A:135:ARG:HH21	1:A:192:PRO:CA	2.29	0.45
1:B: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:B:402:GLY:HA2	1:B:403:PRO:HD3	1.81	0.45
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.32	0.45
1:B:369:ALA:O	1:B:372:MET:HB2	2.16	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:63:PHE:CD1	1:B:63:PHE:C	2.90	0.45
1:A:113:TYR:O	1:A:116:PHE:CD2	2.70	0.45
1:A:120:ALA:O	1:A:123:PRO:HG2	2.16	0.45
1:B:20:PHE:CE2	1:B:148:CYS:HA	2.51	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:A:227:LEU:HA	1:A:227:LEU:HD23	1.88	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:224:PHE:N	1:B:224:PHE:HD1	2.13	0.45
1:B:72:LEU:O	1:B:72:LEU:HG	2.17	0.45
1:B:23:MET:O	1:B:24:GLY:C	2.54	0.45
1:B:362:MET:O	1:B:363:ILE:C	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:279:ALA:HB3	1:B:280:PRO:CD	2.38	0.45
1:A:208:PHE:CD2	1:A:351:LEU:HD13	2.52	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: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:A:12:PHE:C	1:A:14:LEU:N	2.69	0.45
1:A:116:PHE:C	1:A:116:PHE:CD1	2.88	0.45
1:B:213:ALA:O	1:B:216:LEU:N	2.50	0.45
1:A:175:GLY:O	1:A:176:CYS:C	2.55	0.45
1:B:193:SER:O	1:B:194:SER:CB	2.65	0.45
1:B:30:PHE:O	1:B:31:PRO:C	2.55	0.45
1:A:11:MET:HE2	1:A:11:MET:HA	1.99	0.45
1:B:33:TRP:HH2	1:B:95:PHE:CB	2.30	0.44
1:A:104:LEU:O	1:A:108:ILE:HG13	2.17	0.44
1:A:42:LYS:CE	1:A:373:TYR:HB3	2.47	0.44
1:A:325:GLU:O	1:A:326:VAL:C	2.55	0.44
1:B:327:PRO:HG2	1:B:328:PHE:H	1.82	0.44
1:A:75:TYR:CE2	1:A:79:ILE:HD11	2.52	0.44
1:B:236:TYR:OH	1:B:302:ARG:NH1	2.51	0.44
1:B:42:LYS:HB2	1:B:374:GLU:HB2	1.99	0.44
1:A:48:ILE:HG12	1:A:108:ILE:HG12	1.98	0.44
1:B:233:SER:O	1:B:234:CYS:C	2.56	0.44
1:B:116:PHE:C	1:B:118:PHE:N	2.71	0.44
1:A:210:LEU:O	1:A:213:ALA:HB3	2.17	0.44
1:B:263:TYR:N	1:B:263:TYR:HD1	2.15	0.44
1:B:121:GLY:O	1:B:125:VAL:N	2.49	0.44
1:B:38:ASN:CA	1:B:100:GLN:NE2	2.81	0.44
1:B:244:ALA:O	1:B:247:PHE:N	2.51	0.44
1:B:123:PRO:O	1:B:127:ALA:HB2	2.17	0.44
1:A:196:THR:HG21	1:A:201:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:CG1	1:B:178:LEU:HD22	2.47	0.44
1:B:74:LYS:N	1:B:74:LYS:CD	2.72	0.44
1:B:228:TYR:O	1:B:229:VAL: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:246:PHE:CD1	1:A:247:PHE:N	2.83	0.44
1:B:345:PHE:O	1:B:346:SER:C	2.55	0.44
1:B:217:PHE:HD2	1:B:223:TRP:HH2	1.65	0.44
1:B:40:ILE:CG1	1:B:44:ASP:HB2	2.48	0.44
1:B:51:ALA:HB3	1:B:112:ILE:HD11	1.99	0.44
1:A:307:SER:HA	1:A:379:GLN:HB3	1.99	0.44
1:B:337:ILE:O	1:B:341:PHE:HB2	2.17	0.44
1:B:336:TYR:CE2	1:B:400:LEU:HD11	2.52	0.44
1:B:104:LEU:HG	1:B:108:ILE:HD11	1.99	0.44
1:B:38:ASN:CB	1:B:100:GLN:NE2	2.81	0.44
1:B:51:ALA:O	1:B:52:ILE:C	2.55	0.44
1:A:89:PRO:O	1:A:93:PHE:HB2	2.17	0.44
1:A:4:LEU:CD2	1:A:10:TRP:HZ3	2.28	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:B:40:ILE:CD1	1:B:48:ILE:HD12	2.47	0.43
1:A:288:GLY:O	1:A:290:ASN:N	2.51	0.43
1:A:382:TYR:N	1:A:382:TYR:CD1	2.86	0.43
1:A:264:VAL:O	1:A:267:MET:N	2.51	0.43
1:A:177:ALA:O	1:A:181:ALA:CB	2.65	0.43
1:B:139:GLU:C	1:B:141:GLY:N	2.71	0.43
1:B:307:SER:HA	1:B:379:GLN:HB3	2.00	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: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:B:260:VAL:O	1:B:261:PHE:C	2.55	0.43
1:B:391:GLY:O	1:B:395:ILE:HG13	2.18	0.43
1:A:40:ILE:CD1	1:A:48:ILE:HD12	2.49	0.43
1:B:195:ALA:O	1:B:196:THR:CG2	2.60	0.43
1:B:173:GLY:O	1:B:177:ALA:HB2	2.18	0.43
1:B:134:ARG:NH1	1:B:203:ALA:CA	2.80	0.43
1:A:135:ARG:NH2	1:A:192:PRO:C	2.72	0.43
1:B:13:GLY:O	1:B:146:PHE:CD2	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:124:ALA:O	1:B:127:ALA:HB3	2.19	0.43
1:A:188:LYS:HB2	1:A:189:THR:H	1.71	0.43
1:A:55:PHE:CE1	1:A:113:TYR:CE1	3.07	0.43
1:A:295:ALA:O	1:A:298:ILE:HB	2.19	0.43
1:B:320:THR:C	1:B:322:HIS:H	2.22	0.43
1:A:53:SER:O	1:A:56:SER:N	2.48	0.43
1:B:57:LEU:HD13	1:B:355:CYS:O	2.19	0.43
1:B:299:MET:O	1:B:302:ARG:N	2.52	0.43
1:B:11:MET:O	1:B:14:LEU:HB2	2.19	0.43
1:A:9:PHE:CD2	1:A:10:TRP:N	2.87	0.43
1:B:78:TRP:NE1	1:B:185:PHE:CD1	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: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:A:96:GLY:O	1:A:100:GLN:N	2.40	0.43
1:A:18:PHE:CZ	1:A:180:LEU:HD12	2.53	0.43
1:B:78:TRP:O	1:B:80:ILE:N	2.51	0.43
1:B:346:SER:O	1:B:347:ALA:C	2.57	0.43
1:B:90:PHE:CD2	1:B:114:LEU:HD13	2.53	0.43
1:A:26:TYR:O	1:A:27:PHE:C	2.58	0.43
1:A:378:PHE:O	1:A:382:TYR:CD1	2.72	0.43
1:A:325:GLU:O	1:A:326:VAL:O	2.37	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: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:B:319:LYS:O	1:B:321:LEU:N	2.52	0.42
1:B:372:MET:O	1:B:376:ILE:HB	2.19	0.42
1:A:51:ALA:HB3	1:A:112:ILE:HD11	2.00	0.42
1:B:9:PHE:HE2	1:B:10:TRP:CZ3	2.36	0.42
1:A:2:TYR:CE2	1:A:3:TYR:CD2	3.07	0.42
1:B:326:VAL:HB	1:B:327:PRO:HD3	1.93	0.42
1:A:277:PHE:HD2	1:A:278:PHE:HE1	1.67	0.42
1:B:244:ALA:O	1:B:247:PHE:HB3	2.19	0.42
1:A:288:GLY:O	1:A:291:ALA:N	2.52	0.42
1:A:158:VAL:O	1:A:159:GLY:C	2.57	0.42
1:A:246:PHE:HB2	1:A:378:PHE:HD2	1.76	0.42
1:A:370:GLY:HA2	1:A:373:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:CG1	1:A:319:LYS:HG2	2.33	0.42
1:A:320:THR:C	1:A:322:HIS:N	2.73	0.42
1:A:211:LYS:O	1:A:212:LEU:C	2.57	0.42
1:B:369:ALA:O	1:B:370:GLY:C	2.57	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:B:2:TYR:CE2	1:B:3:TYR:CD2	3.07	0.42
1:A:85:VAL:O	1:A:174:SER:OG	2.36	0.42
1:A:154:GLY:O	1:A:157:ILE:N	2.52	0.42
1:A:372:MET:O	1:A:376:ILE:HB	2.20	0.42
1:B:293:LEU:HD22	1:B:397:VAL:CG2	2.50	0.42
1:B:299:MET:O	1:B:303:ILE:HG13	2.20	0.42
1:A: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: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:381:ALA:O	1:B:384:VAL:N	2.53	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:323:MET:HA	1:B:326:VAL:CG2	2.49	0.42
1:A:125:VAL:O	1:A:129:ILE:HG13	2.20	0.42
1:B:54:LEU:HA	1:B:363:ILE:HD11	2.01	0.42
1:B:373:TYR:O	1:B:377:GLY:N	2.44	0.42
1:B:9:PHE:O	1:B:10:TRP:C	2.58	0.42
1:A:260:VAL:O	1:A:264:VAL:HG23	2.19	0.42
1:B:26:TYR:O	1:B:27:PHE:C	2.58	0.42
1:B:99:LEU:O	1:B:102:ASN:N	2.48	0.42
1:B:8:ASN:O	1:B:9:PHE:C	2.55	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:20:PHE:HD2	1:B:151:TRP:CB	2.18	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
1:A:2:TYR:CE2	1:A:3:TYR:HD2	2.37	0.42
1:B:22:ILE:HG13	1:B:22:ILE:H	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:O	1:B:112:ILE:HG13	2.20	0.42
1:B:367:VAL:O	1:B:368:LEU:C	2.57	0.42
1:A:312:ALA:O	1:A:315:VAL:N	2.53	0.42
1:B:168:PHE:O	1:B:171:TRP:N	2.53	0.42
1:A:195:ALA:O	1:A:196:THR:CG2	2.63	0.42
1:A:273:ALA:O	1:A:274:SER:C	2.58	0.42
1:A:72:LEU:O	1:A:72:LEU:HG	2.20	0.42
1:B:250:PHE:CD1	1:B:250:PHE:N	2.88	0.42
1:B:264:VAL:CG1	1:B:319:LYS:HG2	2.37	0.41
1:A:52:ILE:CA	1:A:112:ILE:HD13	2.50	0.41
1:B:60:GLN:HG2	1:B:60:GLN:O	2.19	0.41
1:B:42:LYS:O	1:B:43:SER:C	2.57	0.41
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.50	0.41
1:A:299:MET:SD	1:A:325:GLU:OE2	2.78	0.41
1:A:327:PRO:HG2	1:A:328:PHE:H	1.84	0.41
1:A:10:TRP:HB3	1:A:11:MET:CE	2.49	0.41
1:A:8:ASN:O	1:A:9:PHE:C	2.56	0.41
1:B:85:VAL:HG21	1:B:178:LEU:CD1	2.43	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.87	0.41
1:B:135:ARG:HH21	1:B:192:PRO:CA	2.33	0.41
1:A:90:PHE:CD2	1:A:114:LEU:HD13	2.50	0.41
1:B:351:LEU:HG	1:B:351:LEU:H	1.70	0.41
1:B:107:SER:O	1:B:111:GLY:CA	2.68	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:158:VAL:O	1:B:159:GLY:C	2.58	0.41
1:B:372:MET:O	1:B:376:ILE:N	2.53	0.41
1:B:33:TRP:CE3	1:B:38:ASN:ND2	2.89	0.41
1:A:10:TRP:NE1	1:B:168:PHE:CD1	2.85	0.41
1:B:271:LEU:O	1:B:275:ILE:HG13	2.20	0.41
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.68	0.41
1:A:116:PHE:C	1:A:118:PHE:N	2.73	0.41
1:B:404:GLY:O	1:B:405:PRO:O	2.38	0.41
1:A:193:SER:O	1:A:194:SER:HB3	2.21	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: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:B:370:GLY:O	1:B:371:ASN:C	2.58	0.41
1:A:40:ILE:HD11	1:A:45:THR:N	2.36	0.41
1:A:33:TRP:HH2	1:A:95:PHE:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:O	1:A:341:PHE:HB2	2.21	0.41
1:A:62:LEU:C	1:A:62:LEU:HD12	2.41	0.41
1:B:62:LEU:C	1:B:62:LEU:HD12	2.41	0.41
1:B:359:GLN:OE1	1:B:359:GLN:HA	2.19	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: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:B:40:ILE:HG13	1:B:44:ASP:CB	2.51	0.41
1:B:371:ASN:O	1:B:372:MET:C	2.59	0.41
1:B:381:ALA:O	1:B:382:TYR:C	2.60	0.41
1:A:38:ASN:HA	1:A:100:GLN:NE2	2.36	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:A:14:LEU:O	1:A:15:PHE:C	2.60	0.41
1:B:55:PHE:CZ	1:B:113:TYR:CE1	3.08	0.41
1:A:22:ILE:HG13	1:A:22:ILE:H	1.59	0.41
1:A:277:PHE:HB3	1:A:278:PHE:CD1	2.55	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.89	0.41
1:B:75:TYR:CE2	1:B:79:ILE:HD11	2.56	0.41
1:A:192:PRO:HG2	1:A:197:VAL:HA	2.02	0.41
1:A:248:THR:HG22	1:A:248:THR:O	2.21	0.41
1:B:306:SER:O	1:B:379:GLN:NE2	2.54	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:264:VAL:O	1:B:267:MET:N	2.54	0.40
1:A:31:PRO:O	1:A:34:LEU:HB2	2.22	0.40
1:A:381:ALA:O	1:A:382:TYR:C	2.59	0.40
1:B:188:LYS:HB2	1:B:189:THR:H	1.71	0.40
1:B:55:PHE:HE1	1:B:113:TYR:HH	1.66	0.40
1:A:367:VAL:O	1:A:368:LEU:C	2.60	0.40
1:B:288:GLY:O	1:B:291:ALA:N	2.54	0.40
1:A:20:PHE:N	1:A:20:PHE:CD1	2.85	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:A:236:TYR:OH	1:A:302:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:289:LYS:CG	1:B:400:LEU:HD23	2.24	0.40
1:B:23:MET:O	1:B:24:GLY:O	2.39	0.40
1:A:386:GLY:O	1:A:389:ALA:HB3	2.21	0.40
1:A:275:ILE:CG2	1:A:327:PRO:HG3	2.43	0.40
1:A:216:LEU:CD2	1:A:219:GLN:OE1	2.66	0.40
1:A:387:LEU:O	1:A:388:VAL:C	2.58	0.40
1:B:34:LEU:HD22	1:B:40:ILE:HD12	2.04	0.40
1:A:247:PHE:HD2	1:A:315:VAL:CG1	2.34	0.40
1:A:10:TRP:CZ2	1:B:168:PHE:CD1	3.10	0.40
1:A:179:ILE:O	1:A:183:LEU:HB2	2.22	0.40
1:A:372:MET:O	1:A:376:ILE:N	2.54	0.40
1:B:314:GLU:O	1:B:318:LEU:HG	2.22	0.40
1:B:273:ALA:O	1:B:274:SER:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/417 (100%)	274 (66%)	102 (25%)	39 (9%)	1	10
1	B	415/417 (100%)	271 (65%)	107 (26%)	37 (9%)	1	11
All	All	830/834 (100%)	545 (66%)	209 (25%)	76 (9%)	1	11

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%)	15	52
1	B	345/345 (100%)	317 (92%)	28 (8%)	15	52
All	All	690/690 (100%)	634 (92%)	56 (8%)	15	52

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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