



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1PV6 / pdb_00001pv6
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

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

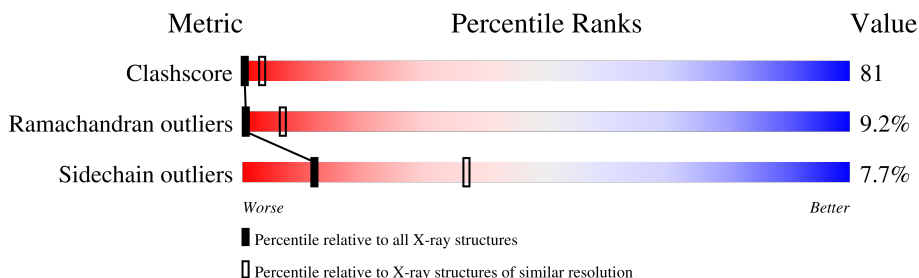
1 Overall quality at a glance

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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	417	17% 65% 17%
1	B	417	19% 63% 18%

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 mutation	UNP P02920
B	154	GLY	CYS	engineered mutation	UNP P02920

F185	F251	V315	S375	L390	V201	F208	L222	L281	L290	C353	C356	F357	K358	Q359	L360	A361	M362	I363	F364	M365	S366	V367	L368	A369	G370	N371	M372	Y373	E374
K188	A252	V316	I376	G391	G202	S209	W223	M276	N290	F354	C355	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374
T189	T253	I317	F377	G392	A203	L210	F224	L271	A291	T348	F357	K358	Q359	L360	A361	M362	I363	F364	M365	S366	V367	L368	A369	G370	N371	M372	Y373	E374	
D190	E255	L318	F378	L391		K211	L225	A272	L292	I349	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
A191	E256	K319	Q379	G390		L212	S226	A273	L293	Y350	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
P192	Q256	T320	A381	A381		A213	L227	S274	L294	L351	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
S193	G257	L321	Y382	A381		L214	E215	I275	L295	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
S194	T258	H322	L383	Y382		E216	L216	S275	L296	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
A195	R259	M323	L384	Y383		L217	F217	I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
T196	F261	E325	V384	L385		L218	R218	I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
V197	G262	V326	L386	G386		L219	Q219	I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
A198	Y263	P327	G386			L220		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	V264	F328	L390	G391		L221		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	T265	L329	G391			L222		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	T266	L330	G391			L223		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	M267	V331	G391			L224		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	G268	G332	G391			L225		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	E269	C333	G391			L226		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L270	F334	G391			L227		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L271	K335	G391			L228		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	N272	Y336	G391			L229		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	A273	I337	G391			L230		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	S274	T338	G391			L231		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	I275	S339	G391			L232		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	M276	Q340	G391			L233		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	F277	F341	G391			L234		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	F278	E342	G391			L235		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	A279	V343	G391			L236		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	P280	R344	G391			L237		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L281	F345	G391			L238		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L282	S346	G391			L239		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L283	A347	G391			L240		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	I286	T348	G391			L241		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	G287	I349	G391			L242		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	G288	Y350	G391			L243		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	G289	L351	G391			L244		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	K289	V352	G391			L245		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	N290	C353	G391			L246		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	A291	F354	G391			L247		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L292	C355	G391			L248		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L293	F356	G391			L249		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L294	F357	G391			L250		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	A295	K358	G391			L251		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	Q296	Q359	G391			L252		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L297	L360	G391			L253		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	I298	A361	G391			L254		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	M299	M362	G391			L255		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	S300	I363	G391			L256		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	V301	F364	G391			L257		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	R302	M365	G391			L258		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L303	S366	G391			L259		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	I304	V367	G391			L260		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	L305	L368	G391			L261		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V366	L367	A368	A369	G370	N371	M372	Y373	E374	
	G306	A369	G391			L262		I276	L297	V352	F356	K357	Q358	L359	A360	M361	I364	M364	S365	V									

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	0.87	1/3387 (0.0%)	1.22	34/4588 (0.7%)
1	B	0.84	1/3387 (0.0%)	1.21	31/4588 (0.7%)
All	All	0.86	2/6774 (0.0%)	1.21	65/9176 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	MET	SD-CE	5.97	1.94	1.79
1	A	197	VAL	CA-CB	5.87	1.61	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	N-CA-C	-10.99	98.97	112.38
1	A	201	VAL	N-CA-C	10.96	123.20	111.58
1	B	114	LEU	N-CA-C	-10.56	99.66	112.54
1	A	190	ASP	N-CA-C	10.43	126.15	113.12
1	B	201	VAL	N-CA-C	9.68	121.84	111.58
1	B	190	ASP	N-CA-C	9.57	125.08	113.12
1	A	251	PHE	N-CA-C	8.86	123.17	110.14
1	B	251	PHE	N-CA-C	8.61	122.80	110.14
1	A	137	ASN	CA-C-N	-7.83	112.65	122.84
1	A	137	ASN	C-N-CA	-7.83	112.65	122.84
1	B	137	ASN	CA-C-N	-7.82	112.37	122.77
1	B	137	ASN	C-N-CA	-7.82	112.37	122.77
1	A	93	PHE	N-CA-C	7.53	121.72	112.23
1	B	138	PHE	N-CA-C	7.50	120.95	108.73
1	B	339	SER	N-CA-C	7.41	119.36	111.28
1	B	93	PHE	N-CA-C	7.40	120.80	111.69
1	A	138	PHE	N-CA-C	7.33	120.73	108.20
1	B	85	VAL	N-CA-C	7.32	118.05	110.36
1	A	19	TYR	N-CA-C	-7.31	101.81	111.24
1	A	56	SER	N-CA-C	-6.87	104.78	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	SER	N-CA-C	-6.72	104.82	113.16
1	B	408	LEU	N-CA-C	6.67	118.34	111.14
1	A	408	LEU	N-CA-C	6.46	118.12	111.14
1	A	197	VAL	N-CA-C	6.40	116.54	110.53
1	B	218	ARG	N-CA-C	-6.39	104.39	111.36
1	A	339	SER	N-CA-C	6.36	118.21	111.28
1	A	140	PHE	N-CA-C	-6.21	104.80	112.38
1	A	85	VAL	N-CA-C	6.20	117.68	110.62
1	A	341	PHE	N-CA-C	6.19	119.58	109.06
1	B	140	PHE	N-CA-C	-6.16	104.86	112.38
1	B	19	TYR	N-CA-C	-6.16	102.13	111.56
1	B	104	LEU	N-CA-C	6.16	121.47	111.37
1	A	352	VAL	N-CA-C	5.94	116.58	110.82
1	A	218	ARG	N-CA-C	-5.88	104.95	111.36
1	B	101	TYR	N-CA-C	-5.87	106.20	113.19
1	B	151	TRP	N-CA-C	-5.85	104.59	110.97
1	B	399	THR	N-CA-C	5.82	121.26	114.04
1	B	8	ASN	N-CA-C	5.79	117.59	111.28
1	A	101	TYR	N-CA-C	-5.78	106.31	113.19
1	B	354	PHE	N-CA-C	5.76	120.43	113.41
1	B	322	HIS	N-CA-C	-5.75	104.70	110.97
1	A	232	VAL	N-CA-C	5.74	115.92	110.53
1	B	341	PHE	N-CA-C	5.64	118.65	109.06
1	B	352	VAL	N-CA-C	5.63	116.28	110.82
1	B	357	PHE	N-CA-C	5.62	121.16	113.97
1	A	357	PHE	N-CA-C	5.59	121.13	113.97
1	B	232	VAL	N-CA-C	5.59	115.78	110.53
1	A	412	GLN	N-CA-C	-5.59	105.72	112.54
1	B	197	VAL	N-CA-C	5.42	115.63	110.53
1	A	96	GLY	CA-C-N	5.41	126.60	119.84
1	A	96	GLY	C-N-CA	5.41	126.60	119.84
1	A	151	TRP	N-CA-C	-5.34	105.15	110.97
1	A	6	ASN	N-CA-C	5.28	117.34	110.43
1	A	60	GLN	N-CA-C	5.25	120.81	113.57
1	B	403	PRO	N-CA-C	-5.24	107.31	113.86
1	A	404	GLY	CA-C-N	5.24	126.39	119.84
1	A	404	GLY	C-N-CA	5.24	126.39	119.84
1	A	184	LEU	N-CA-C	5.20	119.34	112.89
1	B	184	LEU	N-CA-C	5.17	119.31	112.89
1	B	247	PHE	N-CA-C	-5.14	105.17	111.75
1	A	354	PHE	N-CA-C	5.13	119.81	113.50
1	B	209	SER	N-CA-C	5.12	115.97	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	HIS	N-CA-C	-5.10	105.41	110.97
1	A	209	SER	N-CA-C	5.07	115.85	108.14
1	A	399	THR	N-CA-C	5.07	121.60	110.80

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	551	0
1	B	3290	0	3333	529	0
All	All	6580	0	6666	1071	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 81.

All (1071) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:296:GLY:HA2	1:A:299:MET:HE3	1.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:296:GLY:HA2	1:B:299:MET:HE3	1.65	0.79
1:B:163:THR:HG21	1:B:255:GLU:HA	1.65	0.79
1:B:88:ALA:HB3	1:B:89:PRO:HD3	1.65	0.78
1:A:85:VAL:HG22	1:A:178:LEU:HB2	1.66	0.78
1:A:166:ASN:OD1	1:A:167:GLN:N	2.15	0.78
1:B:246:PHE:CD1	1:B:246:PHE:C	2.62	0.78
1:B:1:MET:O	1:B:3:TYR:N	2.15	0.78
1:B:28:PRO:O	1:B:31:PRO:HD2	1.83	0.78
1:A:275:ILE:HG21	1:A:327:PRO:HG3	1.66	0.78
1:A:10:TRP:HE1	1:B:168:PHE:HD1	1.29	0.78
1:A:27:PHE:HB3	1:A:28:PRO:CD	2.13	0.78
1:A:121:GLY:HA2	1:A:124:ALA:HB3	1.65	0.78
1:B:37:ILE:HD13	1:B:166:ASN:HD22	1.48	0.78
1:B:41:SER:O	1:B:45:THR:HG23	1.84	0.78
1:A:251:PHE:CE2	1:A:260:VAL:HG21	2.19	0.78
1:B:85:VAL:HG21	1:B:178:LEU:HD13	1.65	0.77
1:A:74:LYS:HD2	1:A:74:LYS:N	1.97	0.77
1:A:28:PRO:O	1:A:31:PRO:HD2	1.84	0.77
1:B:22:ILE:HB	1:B:118:PHE:CZ	2.19	0.77
1:A:412:GLN:O	1:A:416:VAL:HG23	1.85	0.77
1:B:99:LEU:HD22	1:B:104:LEU:HD12	1.67	0.77
1:B:16:PHE:HE1	1:B:129:ILE:HG21	1.50	0.76
1:B:48:ILE:HA	1:B:108:ILE:HG23	1.65	0.76
1:A:34:LEU:HB3	1:A:40:ILE:CG2	2.15	0.76
1:B:74:LYS:N	1:B:74:LYS:HD2	2.00	0.76
1:B:340:GLN:HE22	1:B:405:PRO:HB3	1.51	0.76
1:B:16:PHE:HB3	1:B:147:GLY:HA3	1.69	0.75
1:B:90:PHE:CE2	1:B:114:LEU:HB3	2.22	0.75
1:B:166:ASN:OD1	1:B:167:GLN:N	2.19	0.75
1:A:16:PHE:HB3	1:A:147:GLY:HA3	1.69	0.75
1:B:33:TRP:O	1:B:37:ILE:HB	1.85	0.75
1:B:34:LEU:HB3	1:B:40:ILE:CG2	2.15	0.75
1:B:412:GLN:O	1:B:416:VAL:HG23	1.86	0.75
1:B:251:PHE:CE2	1:B:260:VAL:HG21	2.22	0.75
1:B:85:VAL:HG22	1:B:178:LEU:HB2	1.69	0.75
1:A:1:MET:O	1:A:4:LEU:N	2.13	0.74
1:A:1:MET:O	1:A:3:TYR:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:O	1:A:196:THR:HG22	1.85	0.74
1:A:234:CYS:SG	1:A:365:MET:SD	2.82	0.74
1:A:1:MET:HB2	1:A:3:TYR:CZ	2.23	0.74
1:A:121:GLY:O	1:A:124:ALA:HB3	1.86	0.74
1:B:27:PHE:HB3	1:B:28:PRO:HD2	1.68	0.74
1:B:87:PHE:HB3	1:B:174:SER:HB2	1.69	0.74
1:B:99:LEU:CD2	1:B:104:LEU:HD12	2.16	0.74
1:B:271:LEU:HD23	1:B:323:MET:HB2	1.69	0.74
1:A:41:SER:O	1:A:45:THR:HG23	1.87	0.74
1:A:246:PHE:CD1	1:A:246:PHE:C	2.66	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:A:44:ASP:HA	1:A:104:LEU:HD21	1.71	0.73
1:A:122:ALA:HB3	1:A:123:PRO:CD	2.18	0.73
1:A:10:TRP:HZ2	1:B:168:PHE:CE1	2.07	0.73
1:B:1:MET:HB2	1:B:3:TYR:CZ	2.23	0.73
1:B:74:LYS:HD2	1:B:74:LYS:H	1.53	0.73
1:B:42:LYS:HZ2	1:B:373:TYR:HB3	1.53	0.73
1:A:172:LEU:HD13	1:B:183:LEU:HD12	1.71	0.72
1:B:230:ILE:HD11	1:B:357:PHE:HB3	1.71	0.72
1:A:22:ILE:HB	1:A:118:PHE:HZ	1.54	0.72
1:B:93:PHE:O	1:B:97:PRO:HG2	1.90	0.72
1:B:163:THR:HG21	1:B:255:GLU:HG3	1.71	0.72
1:B:171:TRP:HA	1:B:171:TRP:CE3	2.24	0.72
1:A:340:GLN:HE22	1:A:405:PRO:HB3	1.54	0.72
1:B:121:GLY:HA2	1:B:124:ALA:HB3	1.71	0.72
1:A:27:PHE:HB3	1:A:28:PRO:HD2	1.71	0.72
1:A:90:PHE:CE2	1:A:114:LEU:HB3	2.24	0.72
1:A:122:ALA:HB3	1:A:123:PRO:HD2	1.71	0.72
1:B:335:LYS:O	1:B:338:THR:HG22	1.89	0.72
1:A:87:PHE:HB3	1:A:174:SER:HB2	1.71	0.72
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.70	0.72
1:B:136:SER:O	1:B:137:ASN:CB	2.38	0.72
1:B:16:PHE:CE1	1:B:129:ILE:HG21	2.25	0.71
1:B:1:MET:O	1:B:4:LEU:N	2.17	0.71
1:B:215:GLU:O	1:B:218:ARG:HB3	1.90	0.71
1:B:122:ALA:HB3	1:B:123:PRO:CD	2.20	0.71
1:A:323:MET:O	1:A:327:PRO:HD2	1.91	0.71
1:A:165:ASN:O	1:A:168:PHE:HB3	1.89	0.71
1:A:338:THR:HG21	1:A:415:GLU:OE2	1.91	0.71
1:B:198:ALA:HB3	1:B:201:VAL:HG23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:ASP:O	1:B:238:VAL:C	2.35	0.69
1:B:415:GLU:OE1	1:B:415:GLU:HA	1.91	0.69
1:A:335:LYS:O	1:A:338:THR:HG22	1.93	0.69
1:A:90:PHE:CZ	1:A:114:LEU:HB3	2.28	0.69
1:A:196:THR:CG2	1:A:201:VAL:HB	2.21	0.69
1:A:215:GLU:O	1:A:218:ARG:HB3	1.93	0.69
1:B:119:ASN:O	1:B:123:PRO:HD2	1.93	0.69
1:A:74:LYS:HD2	1:A:74:LYS:H	1.53	0.69
1:B:90:PHE:CZ	1:B:114:LEU:HB3	2.28	0.69
1:A:66:LEU:O	1:A:70:LEU:HG	1.92	0.69
1:A:22:ILE:HB	1:A:118:PHE:CZ	2.27	0.68
1:A:289:LYS:HA	1:A:400:LEU:HD21	1.74	0.68
1:B:333:CYS:O	1:B:337:ILE:HG13	1.93	0.68
1:B:121:GLY:O	1:B:124:ALA:HB3	1.94	0.68
1:B:16:PHE:CD1	1:B:129:ILE:HD12	2.28	0.68
1:B:171:TRP:HA	1:B:171:TRP:HE3	1.58	0.68
1:B:44:ASP:HA	1:B:104:LEU:HD21	1.75	0.68
1:A:243:PHE:O	1:A:246:PHE:HB3	1.94	0.68
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:A:319:LYS:O	1:A:320:THR:C	2.38	0.67
1:B:37:ILE:HD11	1:B:162:PHE:CE1	2.30	0.67
1:B:198:ALA:HB3	1:B:201:VAL:CG2	2.25	0.67
1:A:9:PHE:HD2	1:A:10:TRP:HE3	1.41	0.67
1:A:171:TRP:HA	1:A:171:TRP:CE3	2.29	0.67
1:A:172:LEU:HD13	1:B:183:LEU:CD1	2.25	0.67
1:A:307:SER:HA	1:A:379:GLN:NE2	2.09	0.67
1:B:16:PHE:CE1	1:B:129:ILE:HD12	2.30	0.67
1:A:216:LEU:HD23	1:A:219:GLN:OE1	1.95	0.66
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.30	0.66
1:B:277:PHE:C	1:B:278:PHE:HD1	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:O	1:A:238:VAL:C	2.38	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:326:VAL:O	1:B:327:PRO:C	2.39	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:A:264:VAL:O	1:A:265:THR:C	2.40	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:A:277:PHE:C	1:A:278:PHE:HD1	2.05	0.65
1:B:289:LYS:HA	1:B:400:LEU:HD21	1.77	0.65
1:A:90:PHE:CD2	1:A:114:LEU:HD22	2.32	0.65
1:B:196:THR:CG2	1:B:201:VAL:HB	2.24	0.65
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.32	0.65
1:A:48:ILE:HA	1:A:108:ILE:CG2	2.27	0.65
1:A:289:LYS:HD3	1:A:403:PRO:HG3	1.77	0.65
1:B:323:MET:SD	1:B:323:MET:N	2.70	0.65
1:A: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:A:7:THR:O	1:A:11:MET:HG2	1.98	0.64
1:B:95:PHE:O	1:B:96:GLY:C	2.40	0.64
1:A:42:LYS:HZ1	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
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:A:83:MET:HE2	1:A:114:LEU:HA	1.80	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:239:PHE:CD1	1:B:239:PHE:C	2.75	0.64
1:B:29:PHE:CE1	1:B:33:TRP:CD1	2.86	0.64
1:B:83:MET:HE2	1:B:114:LEU:HA	1.79	0.64
1:B:283:ILE:HG13	1:B:331:VAL:CG1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:264:VAL:O	1:B:265:THR:C	2.42	0.63
1:A:32:ILE:HD13	1:A:258:THR:HG23	1.79	0.63
1:A:307:SER:HA	1:A:379:GLN:HE21	1.63	0.63
1:B:16:PHE:HB3	1:B:147:GLY:CA	2.29	0.63
1:B:161:MET:HB3	1:B:168:PHE:HE2	1.64	0.63
1:B:307:SER:C	1:B:379:GLN:NE2	2.57	0.63
1:A:34:LEU:HD13	1:A:40:ILE:CD1	2.24	0.63
1:B:390:LEU:C	1:B:390:LEU:HD23	2.24	0.63
1:A:16:PHE:HB3	1:A:147:GLY:CA	2.29	0.62
1:A:16:PHE:CD1	1:A:129:ILE:HD12	2.34	0.62
1:A:279:ALA:O	1:A:283:ILE:HG12	1.98	0.62
1:A: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:90:PHE:CE2	1:B:95:PHE:HE1	2.18	0.62
1:B:323:MET:O	1:B:327:PRO:HD2	1.99	0.62
1:A:85:VAL:HG13	1:A:178:LEU:HB2	1.81	0.62
1:A:154:GLY:O	1:A:155:ALA:C	2.43	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:A:127:ALA:O	1:A:128:PHE:C	2.43	0.62
1:B:63:PHE:CE1	1:B:124:ALA:HB2	2.35	0.61
1:B:268:GLY:HA3	1:B:323:MET:HE2	1.82	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
1:B:20:PHE:HB3	1:B:151:TRP:HB2	1.82	0.61
1:A:121:GLY:C	1:A:124:ALA:HB3	2.26	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:78:TRP:C	1:A:80:ILE:N	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:HG3	1:A:400:LEU:CD2	2.19	0.61
1:B:52:ILE:N	1:B:112:ILE:HD13	2.16	0.61
1:B:177:ALA:O	1:B:181:ALA:HB2	2.00	0.61
1:B:243:PHE:O	1:B:246:PHE:HB3	2.01	0.61
1:B:12:PHE:HE2	1:B:132:VAL:HG21	1.66	0.61
1:A:323:MET:SD	1:A:323:MET:N	2.73	0.61
1:B:246:PHE:HD1	1:B:247:PHE:N	1.99	0.61
1:A:239:PHE:CD1	1:A:239:PHE:C	2.78	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:329:LEU:O	1:B:333:CYS:HB2	2.00	0.60
1:A:239:PHE:HD1	1:A:240:ASP:N	1.99	0.60
1:A:77:LEU:O	1:A:80:ILE:HB	2.01	0.60
1:B:307:SER:HA	1:B:379:GLN:HE21	1.66	0.60
1:A:40:ILE:HD13	1:A:45:THR:HG22	1.83	0.60
1:A:107:SER:O	1:A:111:GLY:N	2.35	0.60
1:A:283:ILE:HG13	1:A:331:VAL:HG11	1.82	0.60
1:B:4:LEU:HD22	1:B:10:TRP:HZ3	1.66	0.60
1:B:116:PHE:C	1:B:118:PHE:H	2.10	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:A:24:GLY:O	1:A:25:ALA:C	2.45	0.60
1:B:239:PHE:C	1:B:239:PHE:HD1	2.09	0.60
1:A:215:GLU:OE1	1:A:215:GLU:C	2.45	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:113:TYR:C	1:A:115:GLY:N	2.55	0.59
1:A:340:GLN:NE2	1:A:405:PRO:HB3	2.17	0.59
1:A:368:LEU:O	1:A:372:MET:HG3	2.02	0.59
1:A:198:ALA:HB3	1:A:201:VAL:HG23	1.84	0.59
1:B:66:LEU:O	1:B:70:LEU:HG	2.01	0.59
1:B:338:THR:CG2	1:B:339:SER:N	2.64	0.59
1:A:98:LEU:HB2	1:A:107:SER:OG	2.03	0.59
1:A:163:THR:CG2	1:A:255:GLU:HG3	2.32	0.59
1:A:307:SER:C	1:A:379:GLN:NE2	2.61	0.59
1:A:323:MET:HA	1:A:326:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:CG2	1:A:339:SER:N	2.64	0.59
1:B:47:ILE:O	1:B:48:ILE:C	2.42	0.59
1:B:246:PHE:C	1:B:246:PHE:HD1	2.09	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:326:VAL:O	1:A:327:PRO:C	2.45	0.59
1:B:283:ILE:HG13	1:B:331:VAL:HG11	1.84	0.59
1:B:348:THR:HA	1:B:351:LEU:HD12	1.85	0.59
1:B:50:ALA:O	1:B:53:SER:HB3	2.03	0.59
1:B:224:PHE:CD2	1:B:399:THR:CG2	2.86	0.59
1:B:225:LEU:HD13	1:B:336:TYR:CE2	2.38	0.59
1:B:239:PHE:HD1	1:B:240:ASP:N	1.99	0.59
1:A:63:PHE:CE1	1:A:124:ALA:HB2	2.38	0.59
1:B:108:ILE:O	1:B:109:VAL:C	2.46	0.59
1:B:276:MET:HA	1:B:279:ALA:HB2	1.83	0.59
1:B:85:VAL:HG13	1:B:178:LEU:HB2	1.85	0.58
1:B:158:VAL:O	1:B:162:PHE:N	2.30	0.58
1:A:78:TRP:C	1:A:80:ILE:H	2.11	0.58
1:B:40:ILE:HG12	1:B:45:THR:HG23	1.85	0.58
1:B:90:PHE:O	1:B:94:ILE:HG13	2.02	0.58
1:B:196:THR:HG21	1:B:201:VAL:CB	2.30	0.58
1:B:253:THR:HG22	1:B:254:GLY:N	2.17	0.58
1:A:90:PHE:CE2	1:A:95:PHE:HE1	2.20	0.58
1:A:239:PHE:HE2	1:A:303:ILE:HA	1.68	0.58
1:A:373:TYR:HE1	1:A:382:TYR:HE1	1.51	0.58
1:B:90:PHE:HD1	1:B:94:ILE:HD12	1.67	0.58
1:A:62:LEU:O	1:A:66:LEU:HG	2.03	0.58
1:A:239:PHE:C	1:A:239:PHE:HD1	2.12	0.58
1:A:76:LEU:HA	1:A:79:ILE:HD12	1.84	0.58
1:B:24:GLY:O	1:B:25:ALA:C	2.44	0.58
1:A:4:LEU:HD22	1:A:10:TRP:CZ3	2.37	0.58
1:A:47:ILE:O	1:A:48:ILE:C	2.47	0.58
1:A:348:THR:HA	1:A:351:LEU:HD12	1.85	0.58
1:B:294:LEU:O	1:B:298:ILE:HG13	2.03	0.58
1:A:410:ARG:O	1:A:413:VAL:HB	2.04	0.58
1:A:127:ALA:O	1:A:130:GLU:N	2.36	0.58
1:A:289:LYS:HA	1:A:400:LEU:CD2	2.34	0.58
1:B:215:GLU:C	1:B:215:GLU:OE1	2.47	0.58
1:A:172:LEU:CD1	1:B:183:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:O	1:A:286:ILE:HG13	2.04	0.58
1:B:20:PHE:HD1	1:B:20:PHE:H	1.52	0.58
1:B:121:GLY:CA	1:B:124:ALA:HB3	2.34	0.58
1:B:319:LYS:O	1:B:320:THR:C	2.46	0.58
1:B:347:ALA:O	1:B:351:LEU:HG	2.04	0.58
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:28:PRO:O	1:B:29:PHE:C	2.46	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:1:MET:O	1:B:2:TYR:C	2.47	0.57
1:B:37:ILE:HD11	1:B:162:PHE:HZ	1.67	0.57
1:A:10:TRP:CZ2	1:B:168:PHE:CE1	2.92	0.57
1:A:415:GLU:HA	1:A:415:GLU:OE1	2.03	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:95:PHE:O	1:A:96:GLY:C	2.46	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:A:116:PHE:C	1:A:118:PHE:H	2.12	0.57
1:B:42:LYS:HG3	1:B:374:GLU:N	2.20	0.57
1:B:55:PHE:O	1:B:59:PHE:HB2	2.04	0.57
1:B:148:CYS:O	1:B:148:CYS:SG	2.63	0.57
1:B:278:PHE:N	1:B:278:PHE:CD1	2.73	0.57
1:A:74:LYS:H	1:A:74:LYS:CD	2.15	0.57
1:A: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:226:SER:O	1:A:227:LEU:C	2.48	0.57
1:A:246:PHE:C	1:A:246:PHE:HD1	2.13	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:382:TYR:O	1:A:383:LEU:C	2.46	0.56
1:A:11:MET:N	1:A:11:MET:HE2	2.21	0.56
1:A:18:PHE:CE1	1:A:180:LEU:HD12	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TYR:HD1	1:B:263:TYR:H	1.53	0.56
1:B:326:VAL:HB	1:B:327:PRO:HD2	1.83	0.56
1:A:25:ALA:HA	1:A:158:VAL:HG21	1.88	0.56
1:A:333:CYS:O	1:A:337:ILE:HG13	2.05	0.56
1:B:208:PHE:HA	1:B:212:LEU:HD12	1.88	0.56
1:A:37:ILE:HD11	1:A:162:PHE:HZ	1.65	0.56
1:A:90:PHE:CB	1:A:114:LEU:HD13	2.36	0.56
1:A:198:ALA:HB3	1:A:201:VAL:CG2	2.36	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CD2	2.24	0.56
1:B:48:ILE:HA	1:B:108:ILE:CG2	2.32	0.56
1:B:226:SER:O	1:B:227:LEU:C	2.49	0.56
1:B:278:PHE:HD1	1:B:278:PHE:N	2.03	0.56
1:A:2:TYR:CE1	1:A:137:ASN:ND2	2.74	0.56
1:A:108:ILE:O	1:A:112:ILE:HG13	2.05	0.56
1:B:17:PHE:HD2	1:B:18:PHE:CE2	2.24	0.56
1:B:44:ASP:O	1:B:48:ILE:HG13	2.06	0.56
1:B:74:LYS:H	1:B:74:LYS:CD	2.16	0.56
1:B:78:TRP:C	1:B:80:ILE:N	2.63	0.56
1:A:332:GLY:O	1:A:333:CYS:C	2.49	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:127:ALA:O	1:B:128:PHE:C	2.45	0.55
1:B:382:TYR:O	1:B:383:LEU:C	2.48	0.55
1:A:1:MET:O	1:A:2:TYR:C	2.49	0.55
1:A:63:PHE:CE2	1:A:76:LEU:HD21	2.41	0.55
1:A:290:ASN:O	1:A:291:ALA:C	2.48	0.55
1:A:12:PHE:O	1:A:15:PHE:N	2.39	0.55
1:A:44:ASP:HA	1:A:104:LEU:CD2	2.36	0.55
1:A:208:PHE:HA	1:A:212:LEU:HD12	1.88	0.55
1:A:338:THR:HG23	1:A:339:SER:N	2.21	0.55
1:A:390:LEU:C	1:A:390:LEU:HD23	2.32	0.55
1:B:50:ALA:HB1	1:B:363:ILE:HA	1.89	0.55
1:B:85:VAL:CG2	1:B:178:LEU:HD13	2.36	0.55
1:B:113:TYR:C	1:B:115:GLY:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLY:O	1:B:289:LYS:C	2.49	0.55
1:A:128:PHE:C	1:A:128:PHE:CD1	2.85	0.55
1:A:315:VAL:O	1:A:316:VAL:C	2.49	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:B:18:PHE:CE1	1:B:180:LEU:HD12	2.41	0.55
1:A:224:PHE:CD1	1:A:224:PHE:N	2.72	0.55
1:A:17:PHE:HD2	1:A:18:PHE:CE2	2.25	0.55
1:A:85:VAL:CG2	1:A:178:LEU:HD13	2.35	0.55
1:B:136:SER:O	1:B:137:ASN:HB2	2.06	0.55
1:A:228:TYR:CZ	1:A:292:LEU:HB3	2.42	0.55
1:A:244:ALA:O	1:A:245:ASN:C	2.50	0.55
1:A:346:SER:OG	1:A:347:ALA:N	2.40	0.55
1:B:44:ASP:HA	1:B:104:LEU:CD2	2.36	0.55
1:B:279:ALA:O	1:B:282:ILE:HB	2.07	0.55
1:B:372:MET:HE1	1:B:384:VAL:CB	2.37	0.55
1:A:28:PRO:O	1:A:29:PHE:C	2.49	0.54
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:A:9:PHE:O	1:A:10:TRP:C	2.50	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:B:290:ASN:O	1:B:291:ALA:C	2.50	0.54
1:A:20:PHE:HB3	1:A:151:TRP:CA	2.37	0.54
1:B:116:PHE:C	1:B:116:PHE:CD1	2.85	0.54
1:B:124:ALA:O	1:B:127:ALA:N	2.39	0.54
1:A:55:PHE:O	1:A:59:PHE:HB2	2.07	0.54
1:A:311:SER:O	1:A:314:GLU:HB3	2.07	0.54
1:B:135:ARG:HH21	1:B:192:PRO:HA	1.71	0.54
1:A:283:ILE:HG13	1:A:331:VAL:HG12	1.90	0.54
1:A:288:GLY:O	1:A:289:LYS:C	2.48	0.54
1:A:336:TYR:OH	1:A:401:SER:HB2	2.07	0.54
1:B:86:MET:C	1:B:89:PRO:HD2	2.32	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:336:TYR:OH	1:A:401:SER:CB	2.56	0.54
1:B:121:GLY:C	1:B:124:ALA:HB3	2.33	0.54
1:B:307:SER:CA	1:B:379:GLN:NE2	2.71	0.54
1:A:25:ALA:O	1:A:26:TYR:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:ILE:HD13	1:B:45:THR:HG22	1.90	0.54
1:A:10:TRP:NE1	1:B:168:PHE:HD1	2.03	0.53
1:A:55:PHE:CZ	1:A:113:TYR:HE1	2.27	0.53
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.90	0.53
1:B:20:PHE:HB3	1:B:151:TRP:CA	2.38	0.53
1:B:125:VAL:O	1:B:129:ILE:HG13	2.08	0.53
1:A:108:ILE:O	1:A:109:VAL:C	2.49	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:141:GLY:O	1:B:145:MET:HG3	2.08	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: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:A:97:PRO:O	1:A:98:LEU:C	2.52	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:B:244:ALA:O	1:B:245:ASN:C	2.52	0.53
1:A:90:PHE:O	1:A:94:ILE:HG13	2.09	0.53
1:A:174:SER:O	1:A:177:ALA:HB3	2.09	0.53
1:B:319:LYS:O	1:B:322:HIS:N	2.31	0.53
1:A:17:PHE:HD2	1:A:18:PHE:CD2	2.27	0.53
1:A:85:VAL:CG2	1:A:178:LEU:HB2	2.38	0.53
1:A:244:ALA:O	1:A:247:PHE:N	2.42	0.53
1:A:369:ALA:O	1:A:370:GLY:C	2.52	0.53
1:B:277:PHE:HD2	1:B:278:PHE:CE1	2.27	0.53
1:B:372:MET:HE1	1:B:384:VAL:HB	1.90	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:B:299:MET:SD	1:B:325:GLU:OE2	2.66	0.52
1:B:116:PHE:O	1:B:118:PHE:N	2.42	0.52
1:B:128:PHE:C	1:B:128:PHE:CD1	2.85	0.52
1:A:116:PHE:O	1:A:118:PHE:N	2.42	0.52
1:B:112:ILE:O	1:B:112:ILE:HG22	2.09	0.52
1:A:135:ARG:O	1:A:135:ARG:HD3	2.10	0.52
1:A:228:TYR:O	1:A:229:VAL:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:MET:O	1:A:363:ILE:C	2.49	0.52
1:B:224:PHE:CD1	1:B:224:PHE:N	2.76	0.52
1:B:239:PHE:HE2	1:B:303:ILE:HA	1.73	0.52
1:A:112:ILE:HG22	1:A:112:ILE:O	2.10	0.52
1:A:329:LEU:O	1:A:330:LEU:C	2.53	0.52
1:B:78:TRP:C	1:B:80:ILE:H	2.17	0.52
1:A:107:SER:O	1:A:111:GLY:HA3	2.08	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:151:TRP:HD1	1:B:269:GLU:HG3	1.73	0.52
1:B:303:ILE:HG21	1:B:386:GLY:CA	2.39	0.52
1:B:373:TYR:HE1	1:B:382:TYR:HE1	1.58	0.52
1:A:411:ARG:O	1:A:414:ASN:HB3	2.10	0.52
1:B:86:MET:O	1:B:89:PRO:HD2	2.10	0.52
1:A:263:TYR:CD1	1:A:263:TYR:N	2.77	0.52
1:A:278:PHE:HD1	1:A:278:PHE:N	2.08	0.52
1:B:11:MET:HE2	1:B:11:MET:N	2.25	0.52
1:B:25:ALA:O	1:B:26:TYR:C	2.52	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:62:LEU:O	1:A:62:LEU:HD12	2.10	0.52
1:A:76:LEU:HD12	1:A:79:ILE:HD12	1.91	0.52
1:A:101:TYR:O	1:A:102:ASN:HB2	2.09	0.52
1:A:151:TRP:HD1	1:A:269:GLU:HG3	1.75	0.52
1:A:271:LEU:HG	1:A:275:ILE:HD11	1.92	0.52
1:A:289:LYS:HD2	1:A:401:SER:O	2.09	0.52
1:A:319:LYS:O	1:A:321:LEU:N	2.43	0.52
1:B:62:LEU:HD12	1:B:62:LEU:O	2.10	0.52
1:B:299:MET:O	1:B:300:SER:C	2.53	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:179:ILE:O	1:B:183:LEU:HB2	2.10	0.51
1:B:263:TYR:N	1:B:263:TYR:CD1	2.77	0.51
1:B:336:TYR:OH	1:B:401:SER:CB	2.58	0.51
1:A:33:TRP:HD1	1:A:37:ILE:HD13	1.75	0.51
1:A:50:ALA:O	1:A:53:SER:HB3	2.10	0.51
1:A:136:SER:O	1:A:137:ASN:HB2	2.10	0.51
1:B:239:PHE:CE2	1:B:303:ILE:HG12	2.45	0.51
1:B:332:GLY:O	1:B:333:CYS:C	2.53	0.51
1:A:1:MET:SD	1:A:3:TYR:OH	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CD2	1:A:10:TRP:CE3	2.98	0.51
1:A:18:PHE:CZ	1:A:180:LEU:CD1	2.94	0.51
1:A:70:LEU:HD11	1:A:76:LEU:HB2	1.92	0.51
1:A:127:ALA:O	1:A:130:GLU:HB3	2.11	0.51
1:B:34:LEU:HD13	1:B:40:ILE:CD1	2.36	0.51
1:A:178:LEU:HG	1:A:179:ILE:N	2.26	0.51
1:A:260:VAL:O	1:A:261:PHE:C	2.50	0.51
1:A:33:TRP:HH2	1:A:95:PHE:HB2	1.76	0.51
1:A:135:ARG:NH2	1:A:192:PRO:HA	2.26	0.51
1:A:345:PHE:O	1:A:346:SER:C	2.54	0.51
1:B:8:ASN:ND2	1:B:189:THR:OG1	2.44	0.51
1:B:40:ILE:HG13	1:B:44:ASP:HB2	1.92	0.51
1:B:154:GLY:O	1:B:155:ALA:C	2.54	0.51
1:A:33:TRP:CD1	1:A:37:ILE:HD13	2.45	0.51
1:A:40:ILE:HG12	1:A:45:THR:HG23	1.92	0.51
1:A:85:VAL:HG22	1:A:178:LEU:CB	2.39	0.51
1:A:323:MET:HA	1:A:326:VAL:CG2	2.40	0.51
1:B:175:GLY:O	1:B:176:CYS:C	2.54	0.51
1:A:42:LYS:NZ	1:A:378:PHE:CE1	2.76	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: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: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:315:VAL:O	1:B:316:VAL:C	2.53	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:A:372:MET:HE1	1:A:384:VAL:CB	2.41	0.50
1:A:40:ILE:HG13	1:A:44:ASP:HB2	1.93	0.50
1:A:113:TYR:O	1:A:116:PHE:HD2	1.94	0.50
1:A:51:ALA:O	1:A:52:ILE:C	2.55	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:A:299:MET:O	1:A:300:SER:C	2.55	0.50
1:B:29:PHE:CE1	1:B:170:PHE:CZ	3.00	0.50
1:B:38:ASN:HB3	1:B:100:GLN:NE2	2.27	0.50
1:B:104:LEU:O	1:B:108:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:HG3	1:B:400:LEU:CD2	2.23	0.50
1:B:303:ILE:O	1:B:306:SER:N	2.41	0.50
1:A: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:63:PHE:CD1	1:B:63:PHE:C	2.90	0.50
1:B:116:PHE:CG	1:B:117:CYS:N	2.79	0.50
1:A:30:PHE:O	1:A:31:PRO:C	2.51	0.49
1:A:336:TYR:CE2	1:A:400:LEU:HD11	2.47	0.49
1:B:4:LEU:HD22	1:B:10:TRP:CZ3	2.46	0.49
1:B:320:THR:C	1:B:322:HIS:N	2.69	0.49
1:B:362:MET:O	1:B:363:ILE:C	2.52	0.49
1:B:370:GLY:O	1:B:373:TYR:HB2	2.11	0.49
1:B:23:MET:O	1:B:24:GLY:C	2.54	0.49
1:B:55:PHE:CZ	1:B:113:TYR:HE1	2.30	0.49
1:B:100:GLN:C	1:B:102:ASN:H	2.17	0.49
1:B:400:LEU:HG	1:B:401:SER:N	2.27	0.49
1:A:11:MET:HE2	1:A:11:MET:HA	1.93	0.49
1:A:42:LYS:O	1:A:43:SER:C	2.55	0.49
1:A:116:PHE:C	1:A:116:PHE:CD1	2.88	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:175:GLY:O	1:A:176:CYS:C	2.55	0.49
1:A:238:VAL:HA	1:A:241:GLN:NE2	2.27	0.49
1:A:12:PHE:C	1:A:14:LEU:N	2.69	0.49
1:A:325:GLU:O	1:A:326:VAL:C	2.55	0.49
1:B:30:PHE:O	1:B:31:PRO:C	2.55	0.49
1:B:76:LEU:CD1	1:B:79:ILE:HD12	2.42	0.49
1:B:90:PHE:CB	1:B:114:LEU:HD13	2.41	0.49
1:A:124:ALA:O	1:A:127:ALA:N	2.45	0.49
1:A:381:ALA:O	1:A:384:VAL:N	2.46	0.49
1:A:34:LEU:HD22	1:A:40:ILE:HD12	1.95	0.49
1:B:116:PHE:C	1:B:118:PHE:N	2.71	0.49
1:B:233:SER:O	1:B:234:CYS:C	2.56	0.49
1:A:161:MET:HB3	1:A:168:PHE:HE2	1.78	0.49
1:B:228:TYR:O	1:B:229:VAL:C	2.55	0.49
1:B:97:PRO:O	1:B:98:LEU:C	2.52	0.49
1:B:99:LEU:HD23	1:B:104:LEU:HA	1.95	0.49
1:B:101:TYR:O	1:B:102:ASN:HB2	2.13	0.49
1:B:230:ILE:O	1:B:234:CYS:HB2	2.13	0.49
1:A:29:PHE:CE1	1:A:170:PHE:CZ	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:OG1	1:A:46:GLY:N	2.44	0.49
1:B:345:PHE:O	1:B:346:SER:C	2.55	0.49
1:B:407:SER:OG	1:B:410:ARG:HB2	2.13	0.49
1:A:224:PHE:N	1:A:224:PHE:HD1	2.09	0.49
1:B:51:ALA:O	1:B:54:LEU:N	2.46	0.49
1:B:289:LYS:O	1:B:293:LEU:HG	2.13	0.49
1:B:51:ALA:O	1:B:52:ILE:C	2.55	0.48
1:B:246:PHE:HB2	1:B:378:PHE:HD2	1.70	0.48
1:A:99:LEU:HG	1:A:107:SER:OG	2.12	0.48
1:A: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:340:GLN:C	1:A:341:PHE:CD1	2.91	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:100:GLN:C	1:B:102:ASN:N	2.72	0.48
1:B:341:PHE:CD2	1:B:349:ILE:HD11	2.49	0.48
1:A:84:LEU:HD21	1:A:117:CYS:HB3	1.95	0.48
1:A:91:PHE:HB3	1:A:170:PHE:CE2	2.47	0.48
1:A:320:THR:O	1:A:322:HIS:N	2.46	0.48
1:A:336:TYR:CZ	1:A:400:LEU:HD11	2.48	0.48
1:A:366:SER:O	1:A:369:ALA:HB3	2.13	0.48
1:B:62:LEU:O	1:B:66:LEU:HG	2.13	0.48
1:A:44:ASP:O	1:A:48:ILE:HG13	2.14	0.48
1:B:283:ILE:HG13	1:B:331:VAL:HG12	1.93	0.48
1:A:22:ILE:HD11	1:A:177:ALA:HB1	1.96	0.48
1:A:93:PHE:N	1:A:93:PHE:CD1	2.81	0.48
1:B:260:VAL:O	1:B:261:PHE:C	2.55	0.48
1:A:113:TYR:C	1:A:115:GLY:H	2.20	0.48
1:A:135:ARG:NH2	1:A:192:PRO:C	2.72	0.48
1:B:121:GLY:HA2	1:B:124:ALA:CB	2.43	0.48
1:A:1:MET:HA	1:A:5:LYS:HE3	1.96	0.48
1:A:55:PHE:CZ	1:A:113:TYR:CE1	3.02	0.48
1:A:239:PHE:CD1	1:A:240:ASP:N	2.82	0.48
1:A:305:GLY:O	1:A:318:LEU:HD11	2.13	0.48
1:A:329:LEU:O	1:A:333:CYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ALA:O	1:B:51:ALA:C	2.57	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:33:TRP:HH2	1:B:95:PHE:HB2	1.79	0.48
1:B:40:ILE:HG12	1:B:41:SER:O	2.14	0.48
1:A:90:PHE:HD1	1:A:94:ILE:HD12	1.68	0.47
1:A:227:LEU:O	1:A:228:TYR:C	2.56	0.47
1:B:136:SER:O	1:B:137:ASN:HB3	2.13	0.47
1:B:346:SER:O	1:B:347:ALA:C	2.57	0.47
1:A:233:SER:O	1:A:234:CYS:C	2.56	0.47
1:A:407:SER:OG	1:A:410:ARG:HB2	2.14	0.47
1:A:346:SER:O	1:A:347:ALA:C	2.57	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:A:211:LYS:O	1:A:212:LEU:C	2.57	0.47
1:A:320:THR:C	1:A:322:HIS:N	2.73	0.47
1:B:152:ALA:O	1:B:266:THR:OG1	2.31	0.47
1:B:405:PRO:O	1:B:407:SER:N	2.48	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:1:MET:HA	1:B:5:LYS:HE3	1.97	0.47
1:B:38:ASN:HA	1:B:100:GLN:NE2	2.30	0.47
1:B:52:ILE:HG12	1:B:112:ILE:HG23	1.95	0.47
1:B:114:LEU:HD23	1:B:114:LEU:O	2.15	0.47
1:B:178:LEU:HG	1:B:179:ILE:N	2.30	0.47
1:B:210:LEU:O	1:B:213:ALA:HB3	2.13	0.47
1:B:245:ASN:O	1:B:248:THR:HB	2.15	0.47
1:B:271:LEU:HG	1:B:275:ILE:HD11	1.96	0.47
1:A:16:PHE:HE1	1:A:129:ILE:CG2	2.24	0.47
1:A:86:MET:C	1:A:89:PRO:HD2	2.40	0.47
1:B:9:PHE:O	1:B:10:TRP:C	2.58	0.47
1:B:25:ALA:O	1:B:29:PHE:CB	2.62	0.47
1:B:70:LEU:HD11	1:B:76:LEU:HB2	1.96	0.47
1:B:91:PHE:HB3	1:B:170:PHE:CE2	2.49	0.47
1:B:93:PHE:CD1	1:B:93:PHE:N	2.82	0.47
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.50	0.47
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:O	1:A:159:GLY:C	2.57	0.47
1:A:212:LEU:HD22	1:A:345:PHE:CE1	2.49	0.47
1:A:223:TRP:HA	1:A:223:TRP:CE3	2.50	0.47
1:A:303:ILE:O	1:A:306:SER:N	2.39	0.47
1:A:400:LEU:HG	1:A:401:SER:N	2.30	0.47
1:A:263:TYR:O	1:A:264:VAL:C	2.58	0.47
1:A:379:GLN:O	1:A:382:TYR:HB2	2.15	0.47
1:B:8:ASN:O	1:B:9:PHE:C	2.55	0.47
1:B:26:TYR:O	1:B:27:PHE:C	2.58	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:116:PHE:CG	1:A:117:CYS:N	2.81	0.46
1:A:235:THR:HG21	1:A:389:ALA:HB2	1.97	0.46
1:A:273:ALA:O	1:A:274:SER:C	2.58	0.46
1:A:372:MET:HE1	1:A:384:VAL:HB	1.95	0.46
1:B:223:TRP:HA	1:B:223:TRP:HE3	1.81	0.46
1:A:37:ILE:CD1	1:A:162:PHE:CZ	2.95	0.46
1:A:122:ALA:C	1:A:124:ALA:N	2.71	0.46
1:A:133:SER:OG	1:A:138:PHE:O	2.33	0.46
1:A:303:ILE:C	1:A:305:GLY:N	2.70	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:B:367:VAL:O	1:B:368:LEU:C	2.57	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:247:PHE:HD2	1:B:315:VAL:CG1	2.27	0.46
1:B:369:ALA:O	1:B:370:GLY:C	2.57	0.46
1:A:9:PHE:HE2	1:A:10:TRP:CZ3	2.34	0.46
1:A:90:PHE:CZ	1:A:95:PHE:HE1	2.34	0.46
1:B:42:LYS:O	1:B:43:SER:C	2.57	0.46
1:B:42:LYS:NZ	1:B:373:TYR:HB3	2.27	0.46
1:B:239:PHE:CD1	1:B:240:ASP:N	2.83	0.46
1:A:11:MET:HE2	1:A:11:MET:CA	2.46	0.46
1:A:26:TYR:O	1:A:27:PHE:C	2.58	0.46
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: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:32:ILE:HD13	1:B:258:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:C	1:B:322:HIS:H	2.22	0.46
1:A:40:ILE:HG12	1:A:41:SER:O	2.16	0.46
1:A:157:ILE:CG2	1:A:161:MET:HG3	2.45	0.46
1:A:223:TRP:HA	1:A:223:TRP:HE3	1.81	0.46
1:B:85:VAL:O	1:B:174:SER:OG	2.34	0.46
1:B:158:VAL:O	1:B:159:GLY:C	2.58	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:178:LEU:O	1:A:179:ILE:C	2.59	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: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:B:307:SER:C	1:B:379:GLN:HE22	2.24	0.46
1:B:370:GLY:O	1:B:371:ASN:C	2.58	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:B:12:PHE:C	1:B:14:LEU:N	2.70	0.45
1:B:62:LEU:HD12	1:B:62:LEU:C	2.41	0.45
1:A:14:LEU:O	1:A:15:PHE:C	2.60	0.45
1:A:139:GLU:C	1:A:141:GLY:N	2.69	0.45
1:A:250:PHE:HD2	1:A:311:SER:C	2.23	0.45
1:B:27:PHE:HB3	1:B:28:PRO:HD3	1.94	0.45
1:B:107:SER:O	1:B:111:GLY:HA3	2.16	0.45
1:B:371:ASN:O	1:B:372:MET:C	2.59	0.45
1:B:381:ALA:O	1:B:382:TYR:C	2.60	0.45
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.32	0.45
1:B:211:LYS:O	1:B:212:LEU:C	2.60	0.45
1:B:402:GLY:HA2	1:B:403:PRO:HD3	1.81	0.45
1:A:50:ALA:O	1:A:51:ALA:C	2.58	0.45
1:A:62:LEU:HD12	1:A:62:LEU:C	2.41	0.45
1:A:367:VAL:O	1:A:368:LEU:C	2.60	0.45
1:A:376:ILE:HG22	1:A:380:GLY:HA3	1.98	0.45
1:A:381:ALA:O	1:A:382:TYR:C	2.59	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:277:PHE:C	1:B:278:PHE:CD1	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:O	1:A:123:PRO:HG2	2.16	0.45
1:A:337:ILE:O	1:A:338:THR:C	2.59	0.45
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.88	0.45
1:A:387:LEU:O	1:A:388:VAL:C	2.58	0.45
1:B:20:PHE:CE2	1:B:148:CYS:HA	2.51	0.45
1:B:72:LEU:HG	1:B:72:LEU:O	2.17	0.45
1:B:224:PHE:N	1:B:224:PHE:HD1	2.13	0.45
1:B:228:TYR:OH	1:B:292:LEU:O	2.33	0.45
1:B:259:ARG:O	1:B:262:GLY:N	2.50	0.45
1:A:20:PHE:HB3	1:A:151:TRP:CB	2.46	0.45
1:A:26:TYR:HD1	1:A:27:PHE:N	2.13	0.45
1:A:172:LEU:O	1:A:176:CYS:SG	2.69	0.45
1:A:208:PHE:CD2	1:A:351:LEU:HD13	2.52	0.45
1:B:273:ALA:O	1:B:274:SER:C	2.59	0.45
1:B:279:ALA:HB3	1:B:280:PRO:CD	2.38	0.45
1:A:8:ASN:O	1:A:9:PHE:C	2.56	0.45
1:A:405:PRO:C	1:A:407:SER:H	2.24	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:42:LYS:CE	1:A:373:TYR:HB3	2.47	0.44
1:A:75:TYR:CE2	1:A:79:ILE:HD11	2.52	0.44
1:A:104:LEU:O	1:A:108:ILE:HG13	2.17	0.44
1:B:33:TRP:HH2	1:B:95:PHE:CB	2.30	0.44
1:B:113:TYR:C	1:B:115:GLY:H	2.23	0.44
1:B:227:LEU:O	1:B:228:TYR:C	2.60	0.44
1:B:327:PRO:HG2	1:B:328:PHE:H	1.82	0.44
1:A:48:ILE:HG12	1:A:108:ILE:HG12	1.98	0.44
1:A:68:ASP:O	1:A:69:LYS:C	2.59	0.44
1:A:210:LEU:O	1:A:213:ALA:HB3	2.17	0.44
1:B:42:LYS:HB2	1:B:374:GLU:HB2	1.99	0.44
1:B:68:ASP:O	1:B:69:LYS:C	2.60	0.44
1:B:236:TYR:OH	1:B:302:ARG:NH1	2.51	0.44
1:B:263:TYR:HD1	1:B:263:TYR:N	2.15	0.44
1:A:100:GLN:C	1:A:102:ASN:H	2.23	0.44
1:B:121:GLY:O	1:B:125:VAL:N	2.49	0.44
1:A:196:THR:HG21	1:A:201:VAL:CG1	2.48	0.44
1:B:38:ASN:CA	1:B:100:GLN:NE2	2.81	0.44
1:B:74:LYS:N	1:B:74:LYS:CD	2.72	0.44

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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:123:PRO:O	1:B:127:ALA:HB2	2.17	0.44
1:B:244:ALA:O	1:B:247:PHE:N	2.51	0.44
1:A:38:ASN:O	1:A:39:HIS:C	2.59	0.44
1:A:246:PHE:CD1	1:A:247:PHE:N	2.83	0.44
1:B:44:ASP:O	1:B:45:THR:C	2.61	0.44
1:B:217:PHE:HD2	1:B:223:TRP:HH2	1.65	0.44
1:B:307:SER:O	1:B:379:GLN:NE2	2.50	0.44
1:A:307:SER:HA	1:A:379:GLN:HB3	1.99	0.44
1:A:370:GLY:O	1:A:371:ASN:C	2.58	0.44
1:B:38:ASN:O	1:B:39:HIS:C	2.59	0.44
1:B:40:ILE:CG1	1:B:44:ASP:HB2	2.48	0.44
1:B:51:ALA:HB3	1:B:112:ILE:HD11	1.99	0.44
1:B:337:ILE:O	1:B:341:PHE:HB2	2.17	0.44
1:A:4:LEU:CD2	1:A:10:TRP:HZ3	2.28	0.44
1:A:89:PRO:O	1:A:93:PHE:HB2	2.17	0.44
1:B:38:ASN:CB	1:B:100:GLN:NE2	2.81	0.44
1:B: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:250:PHE:HD2	1:B:311:SER:C	2.25	0.44
1:B:293:LEU:O	1:B:294:LEU:C	2.61	0.44
1:A:250:PHE:CD1	1:A:250:PHE:N	2.86	0.44
1:B:80:ILE:O	1:B:81:THR:C	2.59	0.44
1:B:236:TYR:HH	1:B:322:HIS:HD1	1.64	0.44
1:B:259:ARG:O	1:B:260:VAL:C	2.61	0.44
1:B:329:LEU:HD12	1:B:329:LEU:HA	1.69	0.44
1:B:337:ILE:O	1:B:338:THR:C	2.61	0.44
1:A:23:MET:O	1:A:24:GLY:C	2.61	0.43
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:53:SER:O	1:A:54:LEU:C	2.61	0.43
1:A:177:ALA:O	1:A:181:ALA:CB	2.65	0.43
1:A:264:VAL:O	1:A:267:MET:N	2.51	0.43
1:A:288:GLY:O	1:A:290:ASN:N	2.51	0.43
1:A:382:TYR:N	1:A:382:TYR:CD1	2.86	0.43
1:B:40:ILE:CD1	1:B:48:ILE:HD12	2.47	0.43
1:A:63:PHE:CD1	1:A:63:PHE:C	2.95	0.43
1:A:85:VAL:CG1	1:A:178:LEU:HD22	2.48	0.43
1:A:293:LEU:O	1:A:294:LEU:C	2.60	0.43
1:A:299:MET:O	1:A:302:ARG:N	2.51	0.43
1:B:307:SER:HA	1:B:379:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:O	1:B:326:VAL:C	2.61	0.43
1:A:100:GLN:C	1:A:102:ASN:N	2.77	0.43
1:B:135:ARG:NH2	1:B:192:PRO:C	2.77	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:13:GLY:O	1:B:146:PHE:CD2	2.70	0.43
1:B:134:ARG:NH1	1:B:203:ALA:CA	2.80	0.43
1:B:139:GLU:C	1:B:141:GLY:N	2.71	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
1:A:55:PHE:CE1	1:A:113:TYR:CE1	3.07	0.43
1:A:80:ILE:O	1:A:81:THR:C	2.62	0.43
1:A:148:CYS:O	1:A:148:CYS:SG	2.76	0.43
1:A:182:VAL:O	1:A:183:LEU:C	2.61	0.43
1:A:188:LYS:HB2	1:A:189:THR:H	1.71	0.43
1:A:295:ALA:O	1:A:298:ILE:HB	2.19	0.43
1:B:124:ALA:O	1:B:127:ALA:HB3	2.19	0.43
1:B:263:TYR:O	1:B:264:VAL:C	2.61	0.43
1:B:373:TYR:HE1	1:B:382:TYR:CE1	2.36	0.43
1:A:53:SER:O	1:A:56:SER:N	2.48	0.43
1:B:57:LEU:HD13	1:B:355:CYS:O	2.19	0.43
1:B:380:GLY:O	1:B:381:ALA:C	2.61	0.43
1:B:405:PRO:C	1:B:407:SER:H	2.26	0.43
1:A:9:PHE:CD2	1:A:10:TRP:N	2.87	0.43
1:A:253:THR:CG2	1:A:254:GLY:N	2.81	0.43
1:B:11:MET:O	1:B:14:LEU:HB2	2.19	0.43
1:B:78:TRP:NE1	1:B:185:PHE:CD1	2.87	0.43
1:B:299:MET:O	1:B:302:ARG:N	2.52	0.43
1:A:18:PHE:CZ	1:A:180:LEU:HD12	2.53	0.43
1:A:96:GLY:O	1:A:100:GLN:N	2.40	0.43
1:A:234:CYS:O	1:A:235:THR:C	2.61	0.43
1:B:23:MET:O	1:B:26:TYR:HB3	2.19	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:B:222:LEU:O	1:B:223:TRP:C	2.62	0.43
1:A:11:MET:O	1:A:14:LEU:HB2	2.19	0.42
1:A:155:ALA:O	1:A:156:SER:C	2.61	0.42
1:A:259:ARG:O	1:A:260:VAL:C	2.61	0.42
1:B:256:GLN:O	1:B:257:GLY:C	2.61	0.42
1:A:2:TYR:CE2	1:A:3:TYR:CD2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:LEU:O	1:A:386:GLY:C	2.60	0.42
1:B:9:PHE:HE2	1:B:10:TRP:CZ3	2.36	0.42
1:B:319:LYS:O	1:B:321:LEU:N	2.52	0.42
1:B:326:VAL:HB	1:B:327:PRO:HD3	1.93	0.42
1:B:372:MET:O	1:B:376:ILE:HB	2.19	0.42
1:A:120:ALA:O	1:A:121:GLY:C	2.62	0.42
1:A:246:PHE:HB2	1:A:378:PHE:HD2	1.76	0.42
1:A:264:VAL:CG1	1:A:319:LYS:HG2	2.33	0.42
1:A:288:GLY:O	1:A:291:ALA:N	2.52	0.42
1:A:370:GLY:HA2	1:A:373:TYR:HD2	1.84	0.42
1:B:244:ALA:O	1:B:247:PHE:HB3	2.19	0.42
1:A:37:ILE:CD1	1:A:162:PHE:HZ	2.32	0.42
1:A:85:VAL:O	1:A:174:SER:OG	2.36	0.42
1:A:91:PHE:CD2	1:A:170:PHE:CZ	3.07	0.42
1:A:154:GLY:O	1:A:157:ILE:N	2.52	0.42
1:A:307:SER:C	1:A:379:GLN:HE22	2.27	0.42
1:A:372:MET:O	1:A:376:ILE:HB	2.20	0.42
1:B:2:TYR:CE2	1:B:3:TYR:CD2	3.07	0.42
1:A:25:ALA:O	1:A:29:PHE:CB	2.67	0.42
1:A:42:LYS:HB2	1:A:374:GLU:HB2	2.00	0.42
1:A:53:SER:OG	1:A:363:ILE:HG13	2.20	0.42
1:A:78:TRP:CD1	1:A:185:PHE:CE1	3.08	0.42
1:A:276:MET:C	1:A:278:PHE:N	2.77	0.42
1:B:113:TYR:O	1:B:116:PHE:CD2	2.70	0.42
1:B:177:ALA:O	1:B:181:ALA:CB	2.68	0.42
1:B:217:PHE:HD2	1:B:223:TRP:CH2	2.37	0.42
1:B:293:LEU:HD22	1:B:397:VAL:CG2	2.50	0.42
1:B:299:MET:O	1:B:303:ILE:HG13	2.20	0.42
1:A:42:LYS:HG3	1:A:374:GLU:CA	2.49	0.42
1:A:125:VAL:O	1:A:129:ILE:HG13	2.20	0.42
1:A:312:ALA:O	1:A:315:VAL:HG23	2.18	0.42
1:B:1:MET:C	1:B:3:TYR:N	2.78	0.42
1:B:20:PHE:O	1:B:24:GLY:N	2.47	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:10:TRP:HB3	1:A:11:MET:HE3	2.02	0.42
1:A:260:VAL:O	1:A:264:VAL:HG23	2.19	0.42
1:A:401:SER:O	1:A:402:GLY:C	2.62	0.42
1:B:14:LEU:O	1:B:15:PHE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HA	1:B:363:ILE:HD11	2.01	0.42
1:B:373:TYR:O	1:B:377:GLY:N	2.44	0.42
1:A:279:ALA:HB3	1:A:280:PRO:CD	2.41	0.42
1:B:78:TRP:O	1:B:80:ILE:N	2.51	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:A:44:ASP:O	1:A:45:THR:C	2.62	0.42
1:B:20:PHE:HD2	1:B:151:TRP:CB	2.18	0.42
1:B:22:ILE:H	1:B:22:ILE:HG13	1.64	0.42
1:B:40:ILE:HD11	1:B:45:THR:N	2.35	0.42
1:B:373:TYR:CE1	1:B:382:TYR:HE1	2.36	0.42
1:A:72:LEU:HG	1:A:72:LEU:O	2.20	0.42
1:A:195:ALA:O	1:A:196:THR:CG2	2.63	0.42
1:A:312:ALA:O	1:A:315:VAL:N	2.53	0.42
1:B:108:ILE:O	1:B:112:ILE:HG13	2.20	0.42
1:B:168:PHE:O	1:B:171:TRP:N	2.53	0.42
1:B:250:PHE:CD1	1:B:250:PHE:N	2.88	0.42
1:A:52:ILE:CA	1:A:112:ILE:HD13	2.50	0.41
1:A:268:GLY:HA3	1:A:323:MET:HE2	2.02	0.41
1:A:303:ILE:O	1:A:304:ILE:C	2.63	0.41
1:A:350:TYR:O	1:A:351:LEU:C	2.61	0.41
1:B:60:GLN:O	1:B:60:GLN:HG2	2.19	0.41
1:B:264:VAL:CG1	1:B:319:LYS:HG2	2.37	0.41
1:B:385:LEU:O	1:B:386:GLY:C	2.63	0.41
1:A:10:TRP:HB3	1:A:11:MET:CE	2.49	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.87	0.41
1:A:152:ALA:O	1:A:266:THR:OG1	2.34	0.41
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.50	0.41
1:A:299:MET:SD	1:A:325:GLU:OE2	2.78	0.41
1:A:327:PRO:HG2	1:A:328:PHE:H	1.84	0.41
1:B:85:VAL:HG21	1:B:178:LEU:CD1	2.43	0.41
1:B:135:ARG:HH21	1:B:192:PRO:CA	2.33	0.41
1:B:383:LEU:O	1:B:384:VAL:C	2.61	0.41
1:A:90:PHE:CD2	1:A:114:LEU:HD13	2.50	0.41
1:A:371:ASN:O	1:A:372:MET:C	2.63	0.41
1:B:175:GLY:C	1:B:177:ALA:N	2.75	0.41
1:B:351:LEU:HG	1:B:351:LEU:H	1.70	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:B:278:PHE:O	1:B:279:ALA:C	2.64	0.41
1:A:10:TRP:NE1	1:B:168:PHE:CD1	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:312:ALA:O	1:A:313:LEU:C	2.62	0.41
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.68	0.41
1:B:33:TRP:CE3	1:B:38:ASN:ND2	2.89	0.41
1:B:271:LEU:O	1:B:275:ILE:HG13	2.20	0.41
1:B:372:MET:O	1:B:376:ILE:N	2.53	0.41
1:B:404:GLY:O	1:B:405:PRO:O	2.38	0.41
1:A:14:LEU:O	1:A:17:PHE:HB3	2.20	0.41
1:A:51:ALA:O	1:A:54:LEU:N	2.54	0.41
1:B:137:ASN:OD1	1:B:137:ASN:O	2.38	0.41
1:B:401:SER:O	1:B:402:GLY:C	2.64	0.41
1:A:33:TRP:HH2	1:A:95:PHE:CB	2.34	0.41
1:A:40:ILE:HD11	1:A:45:THR:N	2.36	0.41
1:A:337:ILE:O	1:A:341:PHE:HB2	2.21	0.41
1:B:359:GLN:OE1	1:B:359:GLN:HA	2.19	0.41
1:A:34:LEU:O	1:A:38:ASN:C	2.64	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:22:ILE:H	1:A:22:ILE:HG13	1.59	0.41
1:A:38:ASN:HA	1:A:100:GLN:NE2	2.36	0.41
1:A:86:MET:O	1:A:90:PHE:CB	2.69	0.41
1:A:133:SER:OG	1:A:138:PHE:C	2.64	0.41
1:A:192:PRO:HG2	1:A:197:VAL:HA	2.02	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.89	0.41
1:A:277:PHE:HB3	1:A:278:PHE:CD1	2.55	0.41
1:B:40:ILE:HG13	1:B:44:ASP:CB	2.51	0.41
1:B:55:PHE:CZ	1:B:113:TYR:CE1	3.08	0.41
1:B:75:TYR:CE2	1:B:79:ILE:HD11	2.56	0.41
1:B:128:PHE:CE1	1:B:132:VAL:HG21	2.56	0.41
1:A:38:ASN:HB3	1:A:100:GLN:NE2	2.36	0.41
1:A:44:ASP:HB3	1:A:104:LEU:CD1	2.51	0.41
1:A:52:ILE:HA	1:A:112:ILE:HD13	2.03	0.41
1:A:257:GLY:O	1:A:258:THR:C	2.64	0.41
1:B:15:PHE:HD1	1:B:184:LEU:HD12	1.84	0.41
1:B:299:MET:HE2	1:B:325:GLU:HG3	2.03	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:175:GLY:C	1:A:177:ALA:N	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:O	1:B:179:ILE:C	2.64	0.40
1:B:188:LYS:HB2	1:B:189:THR:H	1.71	0.40
1:B:264:VAL:O	1:B:267:MET:N	2.54	0.40
1:A:20:PHE:CD1	1:A:20:PHE:N	2.85	0.40
1:A:236:TYR:OH	1:A:302:ARG:NH1	2.54	0.40
1:B:53:SER:O	1:B:54:LEU:C	2.62	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
1:A:1:MET:C	1:A:3:TYR:N	2.79	0.40
1:A:20:PHE:O	1:A:24:GLY:N	2.49	0.40
1:A:302:ARG:O	1:A:302:ARG:HG2	2.20	0.40
1:A:320:THR:C	1:A:322:HIS:H	2.28	0.40
1:B:8:ASN:CG	1:B:189:THR:OG1	2.65	0.40
1:B:25:ALA:O	1:B:29:PHE:HB3	2.21	0.40
1:B:90:PHE:CE2	1:B:95:PHE:CE1	3.04	0.40
1:B:303:ILE:C	1:B:305:GLY:N	2.75	0.40
1:A:216:LEU:CD2	1:A:219:GLN:OE1	2.66	0.40
1:A:222:LEU:O	1:A:223:TRP:C	2.64	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: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:B:348:THR:O	1:B:349:ILE:C	2.64	0.40
1:A:10:TRP:CZ2	1:B:168:PHE:CD1	3.10	0.40
1:A:179:ILE:O	1:A:183:LEU:HB2	2.22	0.40
1:A:247:PHE:HD2	1:A:315:VAL:CG1	2.34	0.40
1:A:372:MET:O	1:A:376:ILE:N	2.54	0.40
1:B:30:PHE:C	1:B:30:PHE:CD1	3.00	0.40
1:B:34:LEU:HD22	1:B:40:ILE:HD12	2.04	0.40
1:B:276:MET:C	1:B:278:PHE:N	2.75	0.40
1:B:314:GLU:O	1:B:318:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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%)	0	6
1	B	415/417 (100%)	271 (65%)	107 (26%)	37 (9%)	0	7
All	All	830/834 (100%)	545 (66%)	209 (25%)	76 (9%)	0	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	318 (92%)	27 (8%)	11	36
1	B	345/345 (100%)	319 (92%)	26 (8%)	12	37
All	All	690/690 (100%)	637 (92%)	53 (8%)	12	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TRP
1	A	22	ILE
1	A	53	SER
1	A	59	PHE
1	A	62	LEU
1	A	107	SER
1	A	116	PHE
1	A	129	ILE
1	A	136	SER
1	A	138	PHE
1	A	163	THR
1	A	171	TRP
1	A	183	LEU
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

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Mol	Chain	Res	Type
1	A	333	CYS
1	A	355	CYS
1	A	379	GLN
1	A	398	PHE
1	A	401	SER
1	B	10	TRP
1	B	22	ILE
1	B	53	SER
1	B	59	PHE
1	B	62	LEU
1	B	107	SER
1	B	116	PHE
1	B	129	ILE
1	B	136	SER
1	B	138	PHE
1	B	163	THR
1	B	171	TRP
1	B	183	LEU
1	B	239	PHE
1	B	241	GLN
1	B	246	PHE
1	B	278	PHE
1	B	280	PRO
1	B	315	VAL
1	B	323	MET
1	B	325	GLU
1	B	333	CYS
1	B	355	CYS
1	B	379	GLN
1	B	398	PHE
1	B	401	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	119	ASN
1	A	137	ASN
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	272	ASN
1	A	290	ASN
1	A	340	GLN
1	A	371	ASN
1	A	379	GLN
1	B	8	ASN
1	B	38	ASN
1	B	60	GLN
1	B	100	GLN
1	B	102	ASN
1	B	119	ASN
1	B	137	ASN
1	B	241	GLN
1	B	242	GLN
1	B	272	ASN
1	B	290	ASN
1	B	340	GLN
1	B	371	ASN
1	B	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.