



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PYP
Title : X-RAY DIFFRACTION STUDY OF INORGANIC PYROPHOSPHATASE FROM BAKER,S YEAST AT THE 3 ANGSTROMS RESOLUTION (RUSSIAN)
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Deposited on : 1983-02-03
Resolution : 3.00 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

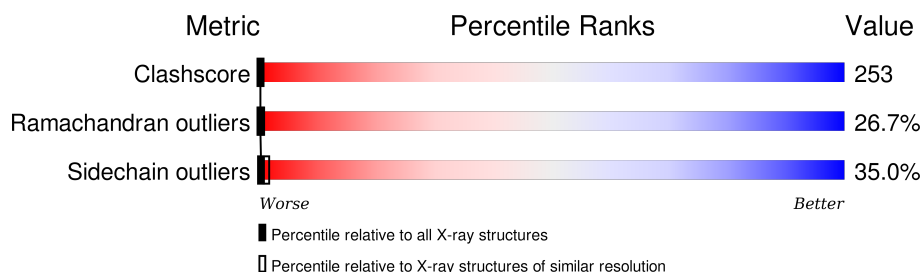
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	285	 6% 38% 39% 16% •
1	B	285	 6% 38% 39% 16% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4472 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 INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	1
			2236	1435	369	429	3			
1	B	281	Total	C	N	O	S	0	0	1
			2236	1435	369	429	3			

There are 18 discrepancies between the modelled and reference sequences:

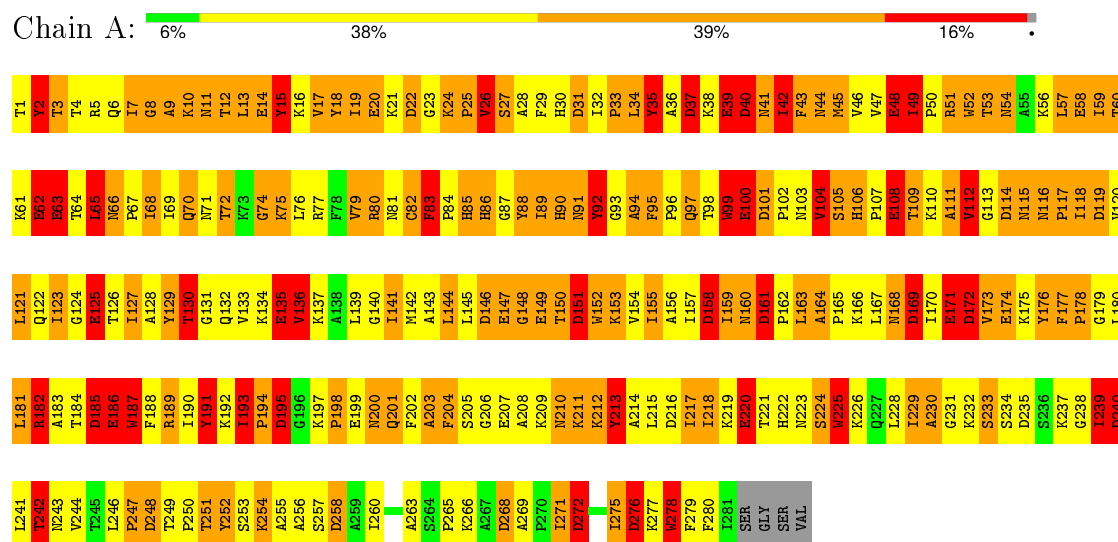
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASP	ASN	CONFLICT	UNP P00817
A	71	ASN	ASP	CONFLICT	UNP P00817
A	?	-	LYS	DELETION	UNP P00817
A	116	ASN	ASP	CONFLICT	UNP P00817
A	122	GLN	GLU	CONFLICT	UNP P00817
A	135	GLU	GLN	CONFLICT	UNP P00817
A	185	ASP	ASN	CONFLICT	UNP P00817
A	223	ASN	ASP	CONFLICT	UNP P00817
A	265	PRO	LEU	CONFLICT	UNP P00817
B	40	ASP	ASN	CONFLICT	UNP P00817
B	71	ASN	ASP	CONFLICT	UNP P00817
B	?	-	LYS	DELETION	UNP P00817
B	116	ASN	ASP	CONFLICT	UNP P00817
B	122	GLN	GLU	CONFLICT	UNP P00817
B	135	GLU	GLN	CONFLICT	UNP P00817
B	185	ASP	ASN	CONFLICT	UNP P00817
B	223	ASN	ASP	CONFLICT	UNP P00817
B	265	PRO	LEU	CONFLICT	UNP P00817

3 Residue-property plots

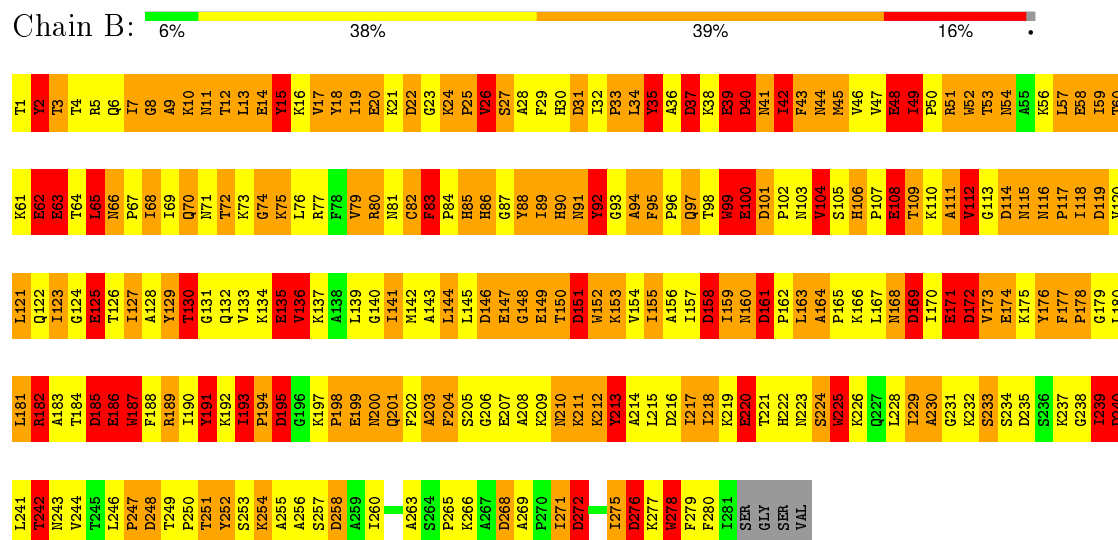
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: INORGANIC PYROPHOSPHATASE



• Molecule 1: INORGANIC PYROPHOSPHATASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α , β , γ	52.23Å 70.29Å 95.47Å 90.00° 90.00° 99.59°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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	1.18	25/2295 (1.1%)	1.40	72/3123 (2.3%)
1	B	1.18	25/2295 (1.1%)	1.40	72/3123 (2.3%)
All	All	1.18	50/4590 (1.1%)	1.40	144/6246 (2.3%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	TRP	NE1-CE2	-7.35	1.28	1.37
1	A	278	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	278	TRP	NE1-CE2	-7.34	1.28	1.37
1	A	99	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	99	TRP	NE1-CE2	-7.33	1.28	1.37
1	B	225	TRP	NE1-CE2	-7.31	1.28	1.37
1	B	187	TRP	NE1-CE2	-7.30	1.28	1.37
1	A	152	TRP	NE1-CE2	-7.29	1.28	1.37
1	A	187	TRP	NE1-CE2	-7.28	1.28	1.37
1	B	52	TRP	NE1-CE2	-7.28	1.28	1.37
1	A	52	TRP	NE1-CE2	-7.26	1.28	1.37
1	B	152	TRP	NE1-CE2	-7.26	1.28	1.37
1	B	220	GLU	CD-OE1	-5.29	1.19	1.25
1	A	220	GLU	CD-OE1	-5.27	1.19	1.25
1	B	62	GLU	CD-OE1	-5.25	1.19	1.25
1	B	48	GLU	CD-OE1	-5.22	1.20	1.25
1	A	174	GLU	CD-OE1	-5.22	1.20	1.25
1	B	20	GLU	CD-OE1	-5.22	1.20	1.25
1	B	125	GLU	CD-OE1	-5.22	1.20	1.25
1	B	186	GLU	CD-OE1	-5.22	1.20	1.25
1	A	62	GLU	CD-OE1	-5.22	1.20	1.25
1	A	20	GLU	CD-OE1	-5.21	1.20	1.25
1	A	186	GLU	CD-OE1	-5.21	1.20	1.25
1	B	199	GLU	CD-OE1	-5.21	1.20	1.25
1	A	48	GLU	CD-OE1	-5.21	1.20	1.25
1	A	199	GLU	CD-OE1	-5.21	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	GLU	CD-OE1	-5.21	1.20	1.25
1	B	147	GLU	CD-OE1	-5.20	1.20	1.25
1	A	149	GLU	CD-OE1	-5.20	1.20	1.25
1	A	125	GLU	CD-OE1	-5.20	1.20	1.25
1	A	207	GLU	CD-OE1	-5.20	1.20	1.25
1	B	149	GLU	CD-OE1	-5.19	1.20	1.25
1	A	100	GLU	CD-OE1	-5.19	1.20	1.25
1	A	147	GLU	CD-OE1	-5.19	1.20	1.25
1	B	63	GLU	CD-OE1	-5.19	1.20	1.25
1	B	14	GLU	CD-OE1	-5.18	1.20	1.25
1	A	39	GLU	CD-OE1	-5.17	1.20	1.25
1	B	100	GLU	CD-OE1	-5.17	1.20	1.25
1	B	108	GLU	CD-OE1	-5.17	1.20	1.25
1	B	135	GLU	CD-OE1	-5.17	1.20	1.25
1	B	39	GLU	CD-OE1	-5.17	1.20	1.25
1	B	207	GLU	CD-OE1	-5.17	1.20	1.25
1	A	63	GLU	CD-OE1	-5.16	1.20	1.25
1	A	108	GLU	CD-OE1	-5.16	1.20	1.25
1	A	14	GLU	CD-OE1	-5.16	1.20	1.25
1	A	58	GLU	CD-OE1	-5.16	1.20	1.25
1	A	135	GLU	CD-OE1	-5.15	1.20	1.25
1	B	171	GLU	CD-OE1	-5.13	1.20	1.25
1	A	171	GLU	CD-OE1	-5.13	1.20	1.25
1	B	58	GLU	CD-OE1	-5.11	1.20	1.25

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ASP	CB-CG-OD1	7.35	124.92	118.30
1	A	172	ASP	CB-CG-OD1	7.35	124.91	118.30
1	B	169	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	158	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	22	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	101	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	258	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	272	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	258	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	235	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	268	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	169	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	151	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	151	ASP	CB-CG-OD1	7.30	124.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	195	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	235	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	22	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	276	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	37	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	40	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	101	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	195	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	119	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	37	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	185	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	216	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	268	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	216	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	158	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	272	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	276	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	248	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	114	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	161	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	161	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	40	ASP	CB-CG-OD1	7.27	124.85	118.30
1	B	185	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	146	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	248	ASP	CB-CG-OD1	7.26	124.84	118.30
1	B	240	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	114	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	240	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	119	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	31	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	31	ASP	CB-CG-OD1	7.23	124.80	118.30
1	B	62	GLU	OE1-CD-OE2	5.86	130.34	123.30
1	B	207	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	207	GLU	OE1-CD-OE2	5.82	130.29	123.30
1	A	20	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	A	62	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	B	135	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	B	186	GLU	OE1-CD-OE2	5.80	130.27	123.30
1	B	63	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	186	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	220	GLU	OE1-CD-OE2	5.80	130.26	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	135	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	B	149	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	B	20	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	220	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	14	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	14	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	B	147	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	A	63	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	147	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	149	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	48	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	171	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	174	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	B	48	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	A	125	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	58	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	39	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	39	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	100	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	174	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	199	GLU	OE1-CD-OE2	5.74	130.18	123.30
1	A	108	GLU	OE1-CD-OE2	5.74	130.18	123.30
1	B	199	GLU	OE1-CD-OE2	5.74	130.18	123.30
1	B	100	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	B	108	GLU	OE1-CD-OE2	5.73	130.17	123.30
1	B	125	GLU	OE1-CD-OE2	5.72	130.16	123.30
1	B	171	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	B	62	GLU	CG-CD-OE2	-5.20	107.91	118.30
1	B	220	GLU	CG-CD-OE2	-5.17	107.95	118.30
1	B	39	GLU	CG-CD-OE2	-5.17	107.95	118.30
1	A	20	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	B	35	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	B	174	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	186	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	62	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	220	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	B	135	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	B	147	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	B	20	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	39	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	171	GLU	CG-CD-OE2	-5.16	107.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	14	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	48	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	63	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	125	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	186	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	58	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	63	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	207	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	48	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	147	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	B	171	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	125	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	135	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	B	108	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	14	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	B	207	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	B	58	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	A	199	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	B	199	GLU	CG-CD-OE2	-5.14	108.03	118.30
1	B	2	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	108	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	100	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	149	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	149	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	A	191	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	191	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	92	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	B	92	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	B	100	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	A	35	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	A	213	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	252	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	B	88	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	18	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	2	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	B	213	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	B	129	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	B	176	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	176	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	18	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	88	TYR	CB-CG-CD1	-5.04	117.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	129	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	B	15	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	15	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2236	0	2198	1132	10
1	B	2236	0	2198	1138	13
All	All	4472	0	4396	2241	13

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 253.

All (2241) 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:1:THR:HG21	1:B:19:ILE:CD1	1.22	1.68
1:B:19:ILE:CD1	1:B:26:VAL:HG11	1.27	1.64
1:A:1:THR:HG21	1:A:19:ILE:CD1	1.22	1.62
1:B:9:ALA:CB	1:B:15:TYR:HB2	1.19	1.61
1:B:42:ILE:HD12	1:B:159:ILE:CD1	1.29	1.60
1:A:190:ILE:HA	1:A:193:ILE:CG1	1.25	1.60
1:A:9:ALA:CB	1:A:15:TYR:HB2	1.19	1.59
1:B:190:ILE:HA	1:B:193:ILE:CG1	1.25	1.59
1:A:19:ILE:CD1	1:A:26:VAL:HG11	1.27	1.58
1:A:105:SER:CB	1:A:112:VAL:HA	1.33	1.56
1:A:42:ILE:HD12	1:A:159:ILE:CD1	1.29	1.56
1:B:1:THR:CG2	1:B:19:ILE:HD11	1.09	1.55
1:B:123:ILE:HD11	1:B:177:PHE:CE2	1.05	1.55
1:B:9:ALA:HB3	1:B:15:TYR:CB	1.33	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:HG23	1:B:221:THR:C	1.22	1.54
1:A:123:ILE:HD11	1:A:177:PHE:CE2	1.05	1.54
1:A:1:THR:CG2	1:A:19:ILE:HD11	1.09	1.53
1:B:105:SER:CB	1:B:112:VAL:HA	1.33	1.53
1:A:95:PHE:CE2	1:A:218:ILE:HD11	1.45	1.52
1:B:222:HIS:NE2	1:B:226:LYS:CE	1.72	1.52
1:A:5:ARG:NH1	1:A:260:ILE:CG2	1.72	1.51
1:A:222:HIS:NE2	1:A:226:LYS:CE	1.72	1.50
1:B:95:PHE:CE2	1:B:218:ILE:HD11	1.45	1.50
1:A:98:THR:HG23	1:A:221:THR:C	1.22	1.50
1:A:9:ALA:HB3	1:A:15:TYR:CB	1.33	1.49
1:A:19:ILE:HD13	1:A:26:VAL:CG1	1.43	1.49
1:B:5:ARG:NH1	1:B:260:ILE:CG2	1.72	1.48
1:B:19:ILE:HD13	1:B:26:VAL:CG1	1.43	1.48
1:B:98:THR:CG2	1:B:221:THR:OG1	1.63	1.46
1:A:5:ARG:HH12	1:A:260:ILE:CG2	1.24	1.46
1:A:123:ILE:CD1	1:A:177:PHE:CE2	1.99	1.45
1:A:98:THR:CG2	1:A:221:THR:OG1	1.63	1.44
1:A:1:THR:CG2	1:A:19:ILE:CD1	1.81	1.44
1:A:139:LEU:HB2	1:A:155:ILE:CG2	1.47	1.44
1:B:139:LEU:HB2	1:B:155:ILE:CG2	1.47	1.44
1:B:123:ILE:CD1	1:B:177:PHE:CE2	1.99	1.42
1:B:49:ILE:CD1	1:B:92:TYR:CD1	2.03	1.42
1:B:5:ARG:HH12	1:B:260:ILE:CG2	1.24	1.42
1:A:123:ILE:CD1	1:A:177:PHE:CD2	2.03	1.40
1:B:123:ILE:CD1	1:B:177:PHE:CD2	2.03	1.40
1:A:49:ILE:CD1	1:A:92:TYR:CD1	2.03	1.40
1:B:123:ILE:HD11	1:B:177:PHE:CD2	1.55	1.39
1:A:7:ILE:CG2	1:A:16:LYS:H	1.37	1.38
1:B:80:ARG:HD2	1:B:279:PHE:CE1	1.59	1.37
1:A:80:ARG:HD2	1:A:279:PHE:CE1	1.59	1.37
1:A:123:ILE:HD11	1:A:177:PHE:CD2	1.55	1.37
1:B:1:THR:CG2	1:B:19:ILE:CD1	1.81	1.36
1:B:23:GLY:O	1:B:24:LYS:CG	1.73	1.36
1:A:174:GLU:O	1:A:178:PRO:CB	1.74	1.35
1:B:5:ARG:NH1	1:B:260:ILE:HG21	1.02	1.35
1:B:83:PHE:CD1	1:B:280:PHE:CE2	2.15	1.35
1:A:105:SER:HB3	1:A:112:VAL:CA	1.58	1.34
1:B:7:ILE:CG2	1:B:16:LYS:H	1.37	1.34
1:A:83:PHE:CD1	1:A:280:PHE:CE2	2.15	1.34
1:A:23:GLY:O	1:A:24:LYS:CG	1.73	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:HB3	1:B:112:VAL:CA	1.58	1.33
1:A:5:ARG:NH1	1:A:260:ILE:HG21	1.02	1.33
1:A:277:LYS:CE	1:B:125:GLU:OE2	1.77	1.32
1:B:49:ILE:HD11	1:B:92:TYR:CD1	1.64	1.32
1:B:112:VAL:O	1:B:150:THR:CB	1.77	1.32
1:A:74:GLY:O	1:A:75:LYS:CG	1.77	1.32
1:B:59:ILE:HG22	1:B:67:PRO:N	1.43	1.32
1:B:98:THR:HG21	1:B:221:THR:CB	1.60	1.32
1:A:59:ILE:HG22	1:A:67:PRO:N	1.43	1.31
1:B:74:GLY:O	1:B:75:LYS:CG	1.77	1.31
1:A:142:MET:CE	1:A:202:PHE:CZ	2.14	1.31
1:B:142:MET:CE	1:B:202:PHE:CZ	2.14	1.31
1:B:174:GLU:O	1:B:178:PRO:CB	1.74	1.31
1:A:52:TRP:N	1:A:88:TYR:O	1.64	1.30
1:A:98:THR:HG21	1:A:221:THR:CB	1.60	1.30
1:A:125:GLU:OE2	1:B:277:LYS:CE	1.77	1.30
1:A:112:VAL:O	1:A:150:THR:CB	1.77	1.29
1:B:52:TRP:N	1:B:88:TYR:O	1.64	1.29
1:B:112:VAL:O	1:B:150:THR:HB	1.11	1.28
1:B:42:ILE:CG1	1:B:43:PHE:H	1.43	1.28
1:A:57:LEU:CA	1:A:68:ILE:O	1.80	1.28
1:A:82:CYS:SG	1:A:190:ILE:HG13	1.73	1.28
1:B:82:CYS:SG	1:B:190:ILE:HG13	1.73	1.28
1:A:53:THR:O	1:A:88:TYR:HB2	1.30	1.28
1:A:27:SER:CA	1:A:64:THR:HG23	1.62	1.28
1:B:53:THR:O	1:B:88:TYR:HB2	1.30	1.28
1:A:42:ILE:CG1	1:A:43:PHE:H	1.44	1.28
1:A:190:ILE:CA	1:A:193:ILE:CG1	2.12	1.27
1:B:27:SER:CA	1:B:64:THR:HG23	1.62	1.27
1:B:83:PHE:CE1	1:B:280:PHE:CE2	2.22	1.27
1:A:58:GLU:HG3	1:A:70:GLN:NE2	1.48	1.27
1:A:49:ILE:HD11	1:A:92:TYR:CD1	1.64	1.27
1:B:57:LEU:CA	1:B:68:ILE:O	1.80	1.26
1:A:112:VAL:O	1:A:150:THR:HB	1.11	1.26
1:A:83:PHE:CE1	1:A:280:PHE:CE2	2.22	1.26
1:B:58:GLU:HG3	1:B:70:GLN:NE2	1.48	1.26
1:B:142:MET:O	1:B:153:LYS:N	1.68	1.25
1:B:190:ILE:CA	1:B:193:ILE:CG1	2.12	1.25
1:A:98:THR:HG23	1:A:221:THR:O	1.14	1.25
1:B:32:ILE:O	1:B:97:GLN:HG3	1.38	1.24
1:B:7:ILE:CG2	1:B:7:ILE:O	1.83	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:O	1:A:153:LYS:N	1.68	1.24
1:A:49:ILE:HD12	1:A:92:TYR:CG	1.73	1.24
1:A:164:ALA:HB3	1:A:165:PRO:CD	1.68	1.23
1:B:98:THR:HG23	1:B:221:THR:O	1.14	1.23
1:B:218:ILE:O	1:B:221:THR:HG22	1.05	1.23
1:A:27:SER:HA	1:A:64:THR:CG2	1.68	1.23
1:B:192:LYS:HB3	1:B:197:LYS:CB	1.67	1.23
1:A:42:ILE:CG2	1:A:137:LYS:HG2	1.69	1.22
1:A:9:ALA:CB	1:A:15:TYR:CB	1.99	1.22
1:B:27:SER:HA	1:B:64:THR:CG2	1.68	1.22
1:A:192:LYS:HB3	1:A:197:LYS:CB	1.67	1.22
1:B:164:ALA:HB3	1:B:165:PRO:CD	1.68	1.22
1:A:163:LEU:CD2	1:A:176:TYR:HD2	1.53	1.22
1:B:49:ILE:HD12	1:B:92:TYR:CG	1.73	1.21
1:B:42:ILE:CG2	1:B:137:LYS:HG2	1.69	1.21
1:A:32:ILE:O	1:A:97:GLN:HG3	1.38	1.21
1:A:100:GLU:O	1:A:114:ASP:O	1.58	1.21
1:A:218:ILE:O	1:A:221:THR:HG22	1.05	1.21
1:A:7:ILE:CG2	1:A:7:ILE:O	1.83	1.21
1:B:9:ALA:CB	1:B:15:TYR:CB	1.99	1.20
1:B:222:HIS:NE2	1:B:226:LYS:HE3	1.37	1.20
1:B:163:LEU:CD2	1:B:176:TYR:HD2	1.53	1.19
1:A:38:LYS:CG	1:A:41:ASN:HB2	1.73	1.19
1:A:193:ILE:HB	1:A:194:PRO:HD3	1.19	1.19
1:B:142:MET:HE3	1:B:202:PHE:CE1	1.77	1.19
1:A:222:HIS:NE2	1:A:226:LYS:HE3	1.37	1.19
1:B:49:ILE:HD12	1:B:92:TYR:CD1	1.73	1.19
1:A:218:ILE:O	1:A:221:THR:CG2	1.91	1.18
1:B:218:ILE:O	1:B:221:THR:CG2	1.91	1.18
1:B:27:SER:CB	1:B:64:THR:HG23	1.73	1.18
1:B:190:ILE:HA	1:B:193:ILE:CD1	1.75	1.17
1:A:27:SER:CB	1:A:64:THR:HG23	1.73	1.17
1:B:100:GLU:O	1:B:114:ASP:O	1.58	1.17
1:B:98:THR:CG2	1:B:221:THR:C	2.12	1.17
1:A:5:ARG:NH2	1:A:25:PRO:HB3	1.59	1.17
1:A:51:ARG:HG2	1:A:89:ILE:HA	1.26	1.17
1:B:9:ALA:HB1	1:B:15:TYR:HB2	1.21	1.17
1:B:10:LYS:HG3	1:B:268:ASP:OD2	1.44	1.17
1:A:7:ILE:HG21	1:A:16:LYS:H	1.02	1.17
1:A:10:LYS:HG3	1:A:268:ASP:OD2	1.44	1.17
1:B:38:LYS:CG	1:B:41:ASN:HB2	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:CG2	1:A:221:THR:C	2.12	1.17
1:B:142:MET:HE3	1:B:202:PHE:CZ	1.77	1.17
1:A:49:ILE:HD12	1:A:92:TYR:CD1	1.73	1.16
1:A:163:LEU:HD21	1:A:176:TYR:HD2	1.07	1.16
1:A:190:ILE:HA	1:A:193:ILE:CD1	1.75	1.16
1:A:42:ILE:HG13	1:A:136:VAL:O	1.00	1.16
1:A:42:ILE:HG12	1:A:43:PHE:N	1.14	1.16
1:B:74:GLY:O	1:B:75:LYS:HG3	1.00	1.16
1:A:164:ALA:HB3	1:A:165:PRO:HD3	1.26	1.15
1:A:74:GLY:O	1:A:75:LYS:HG3	1.00	1.15
1:A:7:ILE:HB	1:A:16:LYS:O	1.47	1.15
1:B:110:LYS:O	1:B:112:VAL:N	1.80	1.15
1:B:5:ARG:NH2	1:B:25:PRO:HB3	1.59	1.15
1:A:110:LYS:O	1:A:112:VAL:N	1.80	1.15
1:B:193:ILE:HB	1:B:194:PRO:HD3	1.19	1.15
1:A:83:PHE:CD1	1:A:280:PHE:CD2	2.35	1.14
1:B:34:LEU:O	1:B:43:PHE:HB3	1.46	1.14
1:B:97:GLN:OE1	1:B:222:HIS:CE1	2.00	1.14
1:B:174:GLU:O	1:B:178:PRO:HB3	0.96	1.14
1:A:27:SER:HA	1:A:64:THR:HG23	1.14	1.14
1:B:42:ILE:HG13	1:B:136:VAL:O	1.00	1.14
1:A:97:GLN:OE1	1:A:222:HIS:CE1	2.00	1.14
1:A:34:LEU:O	1:A:43:PHE:HB3	1.46	1.14
1:B:190:ILE:CA	1:B:193:ILE:HG13	1.76	1.14
1:B:26:VAL:CG2	1:B:27:SER:H	1.57	1.14
1:A:5:ARG:HB3	1:A:263:ALA:HB2	1.20	1.14
1:A:127:ILE:HG22	1:A:128:ALA:N	1.49	1.14
1:B:83:PHE:CD1	1:B:280:PHE:CD2	2.35	1.14
1:A:26:VAL:CG2	1:A:27:SER:H	1.57	1.14
1:B:163:LEU:HD21	1:B:176:TYR:HD2	1.07	1.14
1:A:142:MET:CB	1:A:153:LYS:HB2	1.78	1.13
1:A:69:ILE:O	1:A:70:GLN:O	1.65	1.13
1:A:42:ILE:CG1	1:A:136:VAL:O	1.95	1.13
1:A:193:ILE:HB	1:A:194:PRO:CD	1.76	1.13
1:B:193:ILE:HB	1:B:194:PRO:CD	1.76	1.13
1:A:139:LEU:CB	1:A:155:ILE:HG21	1.78	1.13
1:B:4:THR:HB	1:B:19:ILE:HA	1.29	1.13
1:A:42:ILE:CD1	1:A:159:ILE:CD1	2.25	1.13
1:A:42:ILE:CG1	1:A:43:PHE:N	2.04	1.13
1:A:190:ILE:CA	1:A:193:ILE:HG13	1.76	1.13
1:B:42:ILE:CG1	1:B:136:VAL:O	1.95	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:O	1:B:8:GLY:O	1.65	1.13
1:A:7:ILE:O	1:A:8:GLY:O	1.65	1.13
1:B:142:MET:CE	1:B:202:PHE:CE1	2.32	1.12
1:B:139:LEU:CB	1:B:155:ILE:HG21	1.78	1.12
1:A:135:GLU:O	1:A:136:VAL:HB	1.49	1.12
1:A:142:MET:HE3	1:A:202:PHE:CZ	1.80	1.12
1:A:142:MET:CE	1:A:202:PHE:CE1	2.32	1.12
1:B:42:ILE:CD1	1:B:159:ILE:CD1	2.25	1.12
1:A:174:GLU:O	1:A:178:PRO:HB3	0.96	1.12
1:B:95:PHE:CE2	1:B:218:ILE:CD1	2.33	1.12
1:A:225:TRP:CZ3	1:A:226:LYS:HG2	1.85	1.11
1:B:51:ARG:HG2	1:B:89:ILE:HA	1.26	1.11
1:B:142:MET:CB	1:B:153:LYS:HB2	1.78	1.11
1:A:7:ILE:O	1:A:7:ILE:HG22	1.30	1.11
1:B:222:HIS:NE2	1:B:226:LYS:HE2	1.46	1.11
1:A:95:PHE:CE2	1:A:218:ILE:CD1	2.33	1.11
1:B:42:ILE:CG1	1:B:43:PHE:N	2.04	1.11
1:B:5:ARG:HB3	1:B:263:ALA:HB2	1.20	1.11
1:A:42:ILE:CD1	1:A:159:ILE:HD11	1.81	1.11
1:A:26:VAL:O	1:A:64:THR:HG21	1.51	1.11
1:A:4:THR:HB	1:A:19:ILE:HA	1.28	1.11
1:A:190:ILE:HA	1:A:193:ILE:HG13	1.11	1.11
1:A:200:ASN:O	1:A:201:GLN:HG3	1.49	1.11
1:B:275:ILE:O	1:B:277:LYS:N	1.84	1.11
1:B:42:ILE:CD1	1:B:159:ILE:HD11	1.81	1.10
1:A:97:GLN:OE1	1:A:222:HIS:HE1	1.30	1.10
1:A:275:ILE:O	1:A:277:LYS:N	1.84	1.10
1:A:68:ILE:HG22	1:A:69:ILE:H	1.14	1.10
1:B:127:ILE:CG2	1:B:128:ALA:H	1.63	1.10
1:B:57:LEU:HA	1:B:68:ILE:O	0.94	1.10
1:B:144:LEU:CD2	1:B:153:LYS:HD3	1.81	1.10
1:A:127:ILE:CG2	1:A:128:ALA:H	1.64	1.10
1:B:200:ASN:O	1:B:201:GLN:HG3	1.49	1.10
1:B:68:ILE:HG22	1:B:69:ILE:H	1.14	1.10
1:B:7:ILE:HB	1:B:16:LYS:O	1.47	1.10
1:A:13:LEU:HD23	1:A:76:LEU:HD11	1.26	1.10
1:A:57:LEU:HA	1:A:68:ILE:O	0.94	1.10
1:A:9:ALA:HB1	1:A:15:TYR:HB2	1.21	1.10
1:B:103:ASN:O	1:B:104:VAL:HB	1.37	1.10
1:A:222:HIS:NE2	1:A:226:LYS:HE2	1.46	1.10
1:A:103:ASN:O	1:A:104:VAL:HB	1.37	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HG2	1:B:41:ASN:HB2	1.33	1.09
1:B:26:VAL:O	1:B:64:THR:HG21	1.51	1.09
1:A:19:ILE:CD1	1:A:26:VAL:CG1	2.12	1.09
1:B:69:ILE:O	1:B:70:GLN:O	1.65	1.09
1:B:191:TYR:CE2	1:B:192:LYS:CG	2.36	1.09
1:B:7:ILE:HG21	1:B:16:LYS:H	1.02	1.09
1:B:97:GLN:OE1	1:B:222:HIS:HE1	1.30	1.09
1:B:225:TRP:CZ3	1:B:226:LYS:HG2	1.85	1.09
1:A:142:MET:HE3	1:A:202:PHE:CE1	1.85	1.09
1:B:127:ILE:HG22	1:B:128:ALA:N	1.49	1.09
1:B:190:ILE:HA	1:B:193:ILE:HG13	1.11	1.09
1:A:45:MET:HE1	1:A:120:VAL:HG12	1.31	1.09
1:A:42:ILE:HD12	1:A:159:ILE:HD12	1.13	1.09
1:B:26:VAL:HG22	1:B:27:SER:N	1.62	1.09
1:B:96:PRO:O	1:B:97:GLN:HB2	1.52	1.09
1:B:13:LEU:HD23	1:B:76:LEU:HD11	1.26	1.08
1:B:49:ILE:HD11	1:B:92:TYR:HD1	0.94	1.08
1:A:144:LEU:CD2	1:A:153:LYS:HD3	1.81	1.08
1:B:13:LEU:HD23	1:B:76:LEU:CD1	1.82	1.08
1:B:98:THR:CG2	1:B:221:THR:O	2.01	1.08
1:B:42:ILE:HG12	1:B:43:PHE:N	1.14	1.08
1:A:13:LEU:HD23	1:A:76:LEU:CD1	1.82	1.08
1:A:191:TYR:CE2	1:A:192:LYS:CG	2.36	1.08
1:A:4:THR:CB	1:A:19:ILE:HA	1.83	1.08
1:A:51:ARG:HH11	1:A:51:ARG:HB3	1.03	1.08
1:A:163:LEU:CD2	1:A:176:TYR:CD2	2.36	1.08
1:B:164:ALA:HB3	1:B:165:PRO:HD3	1.26	1.08
1:A:98:THR:CG2	1:A:221:THR:O	2.01	1.08
1:A:49:ILE:HD11	1:A:92:TYR:HD1	0.95	1.08
1:B:51:ARG:HB3	1:B:51:ARG:HH11	1.03	1.08
1:B:163:LEU:CD2	1:B:176:TYR:CD2	2.36	1.08
1:B:191:TYR:CE2	1:B:192:LYS:HG2	1.88	1.08
1:B:19:ILE:CD1	1:B:26:VAL:CG1	2.12	1.07
1:B:4:THR:CB	1:B:19:ILE:HA	1.83	1.07
1:B:29:PHE:CZ	1:B:99:TRP:HD1	1.73	1.07
1:B:42:ILE:HD12	1:B:159:ILE:HD12	1.14	1.07
1:B:12:THR:O	1:B:13:LEU:HG	1.55	1.07
1:A:91:ASN:O	1:A:92:TYR:HB2	1.51	1.07
1:A:96:PRO:O	1:A:97:GLN:HB2	1.53	1.07
1:B:135:GLU:O	1:B:136:VAL:HB	1.49	1.07
1:B:91:ASN:O	1:B:92:TYR:HB2	1.51	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG22	1:A:27:SER:N	1.62	1.06
1:B:1:THR:N	1:B:133:VAL:HG11	1.70	1.06
1:A:191:TYR:CE2	1:A:192:LYS:HG2	1.88	1.06
1:A:9:ALA:O	1:A:10:LYS:HB2	1.50	1.06
1:B:190:ILE:HA	1:B:193:ILE:HG12	1.35	1.06
1:B:7:ILE:HG22	1:B:7:ILE:O	1.30	1.06
1:A:12:THR:O	1:A:13:LEU:HG	1.55	1.06
1:A:190:ILE:HA	1:A:193:ILE:HG12	1.35	1.06
1:B:42:ILE:HG21	1:B:137:LYS:HG2	1.07	1.06
1:A:125:GLU:OE2	1:B:277:LYS:HE3	1.50	1.06
1:A:1:THR:N	1:A:133:VAL:HG11	1.70	1.05
1:A:136:VAL:HA	1:A:159:ILE:HG13	1.36	1.05
1:B:144:LEU:HD21	1:B:153:LYS:HD3	1.07	1.05
1:A:38:LYS:HG2	1:A:41:ASN:HB2	1.33	1.05
1:A:51:ARG:HH11	1:A:51:ARG:CB	1.70	1.05
1:A:192:LYS:HD3	1:A:197:LYS:HD3	1.37	1.05
1:B:27:SER:HB2	1:B:64:THR:HG23	1.35	1.05
1:A:34:LEU:O	1:A:43:PHE:CB	2.04	1.05
1:B:27:SER:HA	1:B:64:THR:HG23	1.15	1.05
1:B:51:ARG:CB	1:B:51:ARG:HH11	1.70	1.05
1:A:29:PHE:CZ	1:A:99:TRP:HD1	1.73	1.05
1:A:65:LEU:O	1:A:66:ASN:ND2	1.90	1.05
1:A:277:LYS:HE3	1:B:125:GLU:OE2	1.50	1.04
1:B:65:LEU:O	1:B:66:ASN:ND2	1.90	1.04
1:B:45:MET:HE1	1:B:120:VAL:HG12	1.39	1.04
1:B:9:ALA:O	1:B:10:LYS:HB2	1.50	1.04
1:B:51:ARG:HG3	1:B:90:HIS:H	1.21	1.04
1:A:83:PHE:HD1	1:A:280:PHE:CD2	1.74	1.04
1:B:34:LEU:O	1:B:43:PHE:CB	2.04	1.04
1:B:155:ILE:O	1:B:155:ILE:HG22	1.56	1.04
1:A:144:LEU:HD21	1:A:153:LYS:HD3	1.07	1.04
1:B:136:VAL:HA	1:B:159:ILE:HG13	1.36	1.04
1:A:49:ILE:O	1:A:91:ASN:O	1.77	1.03
1:A:95:PHE:CD2	1:A:218:ILE:HD11	1.93	1.03
1:B:129:TYR:HB2	1:B:132:GLN:OE1	1.13	1.03
1:B:192:LYS:HB3	1:B:197:LYS:HB2	1.05	1.03
1:B:56:LYS:NZ	1:B:70:GLN:OE1	1.91	1.03
1:A:191:TYR:CD2	1:A:192:LYS:HG3	1.94	1.03
1:A:192:LYS:HB3	1:A:197:LYS:HB2	1.05	1.03
1:A:1:THR:O	1:A:2:TYR:HB2	1.56	1.03
1:A:26:VAL:HG22	1:A:27:SER:H	0.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:NZ	1:A:70:GLN:OE1	1.91	1.03
1:B:1:THR:O	1:B:2:TYR:HB2	1.56	1.03
1:A:42:ILE:HG21	1:A:137:LYS:HG2	1.07	1.03
1:B:123:ILE:O	1:B:123:ILE:CG1	2.07	1.03
1:B:192:LYS:HD3	1:B:197:LYS:HD3	1.37	1.02
1:A:27:SER:HB2	1:A:64:THR:HG23	1.35	1.02
1:B:222:HIS:CD2	1:B:226:LYS:HE3	1.93	1.02
1:A:222:HIS:CD2	1:A:226:LYS:HE3	1.93	1.02
1:A:13:LEU:CD2	1:A:76:LEU:CD1	2.37	1.02
1:A:50:PRO:HB3	1:A:128:ALA:HB3	1.39	1.02
1:B:7:ILE:CG2	1:B:16:LYS:N	2.22	1.02
1:B:80:ARG:HG3	1:B:194:PRO:HB2	1.42	1.02
1:B:95:PHE:CD2	1:B:218:ILE:HD11	1.93	1.02
1:B:42:ILE:HD12	1:B:159:ILE:HD11	1.03	1.02
1:A:136:VAL:CG1	1:A:156:ALA:HB1	1.90	1.01
1:A:48:GLU:O	1:A:49:ILE:HG12	1.59	1.01
1:B:142:MET:HB3	1:B:153:LYS:HB2	1.42	1.01
1:A:80:ARG:HG3	1:A:194:PRO:HB2	1.42	1.01
1:A:51:ARG:HG3	1:A:90:HIS:H	1.21	1.01
1:A:204:PHE:O	1:A:206:GLY:N	1.93	1.01
1:A:42:ILE:HD12	1:A:159:ILE:HD11	1.03	1.01
1:B:137:LYS:HG3	1:B:159:ILE:HG12	1.40	1.01
1:B:13:LEU:CD2	1:B:76:LEU:CD1	2.37	1.01
1:B:50:PRO:HB3	1:B:128:ALA:HB3	1.39	1.01
1:B:57:LEU:HD13	1:B:57:LEU:N	1.74	1.01
1:B:49:ILE:O	1:B:91:ASN:O	1.76	1.01
1:A:137:LYS:HG3	1:A:159:ILE:HG12	1.40	1.01
1:B:244:VAL:HA	1:B:252:TYR:CD1	1.96	1.01
1:A:200:ASN:O	1:A:201:GLN:CG	2.08	1.01
1:B:191:TYR:CD2	1:B:192:LYS:HG3	1.94	1.01
1:B:26:VAL:HG22	1:B:27:SER:H	0.88	1.01
1:A:125:GLU:OE2	1:B:277:LYS:HE2	1.58	1.01
1:B:48:GLU:O	1:B:49:ILE:HG12	1.59	1.01
1:A:155:ILE:O	1:A:155:ILE:HG22	1.56	1.01
1:B:23:GLY:O	1:B:24:LYS:HG3	0.83	1.01
1:A:244:VAL:HA	1:A:252:TYR:CD1	1.96	1.00
1:A:7:ILE:CG2	1:A:16:LYS:N	2.22	1.00
1:A:71:ASN:O	1:A:72:THR:OG1	1.79	1.00
1:A:62:GLU:O	1:A:63:GLU:HB2	1.60	1.00
1:B:136:VAL:CG1	1:B:156:ALA:HB1	1.90	1.00
1:A:139:LEU:CB	1:A:155:ILE:CG2	2.37	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:O	1:A:24:LYS:HG3	0.83	1.00
1:B:83:PHE:HD1	1:B:280:PHE:CD2	1.74	1.00
1:A:123:ILE:CG1	1:A:123:ILE:O	2.07	1.00
1:A:109:THR:HG23	1:A:150:THR:OG1	1.61	1.00
1:A:84:PRO:O	1:A:85:HIS:CG	2.15	1.00
1:B:9:ALA:CB	1:B:15:TYR:CA	2.39	1.00
1:B:109:THR:HG23	1:B:150:THR:OG1	1.61	1.00
1:A:129:TYR:HB2	1:A:132:GLN:OE1	1.13	1.00
1:B:158:ASP:O	1:B:161:ASP:N	1.95	1.00
1:B:200:ASN:O	1:B:201:GLN:CG	2.08	1.00
1:B:84:PRO:O	1:B:85:HIS:CG	2.15	1.00
1:B:139:LEU:CB	1:B:155:ILE:CG2	2.37	1.00
1:A:277:LYS:HE2	1:B:125:GLU:OE2	1.58	0.99
1:A:129:TYR:CB	1:A:132:GLN:OE1	2.10	0.99
1:A:142:MET:HB3	1:A:153:LYS:HB2	1.42	0.99
1:A:172:ASP:O	1:A:174:GLU:N	1.95	0.99
1:B:90:HIS:O	1:B:91:ASN:HB2	1.60	0.99
1:B:204:PHE:O	1:B:206:GLY:N	1.93	0.99
1:A:17:VAL:HG21	1:A:67:PRO:HG2	1.43	0.99
1:B:129:TYR:CB	1:B:132:GLN:OE1	2.10	0.99
1:B:5:ARG:HH11	1:B:260:ILE:HG21	1.17	0.99
1:A:9:ALA:CB	1:A:15:TYR:CA	2.39	0.99
1:A:90:HIS:O	1:A:91:ASN:HB2	1.60	0.99
1:B:115:ASN:O	1:B:116:ASN:O	1.81	0.99
1:B:68:ILE:HG22	1:B:69:ILE:N	1.75	0.99
1:A:158:ASP:O	1:A:161:ASP:N	1.95	0.99
1:A:163:LEU:HD23	1:A:176:TYR:CD2	1.98	0.99
1:A:80:ARG:CD	1:A:279:PHE:CE1	2.46	0.99
1:B:62:GLU:O	1:B:63:GLU:HB2	1.60	0.99
1:B:110:LYS:C	1:B:112:VAL:H	1.66	0.99
1:A:29:PHE:HZ	1:A:99:TRP:CD1	1.81	0.98
1:B:71:ASN:O	1:B:72:THR:OG1	1.79	0.98
1:A:69:ILE:HG21	1:A:76:LEU:HB3	1.45	0.98
1:B:29:PHE:HZ	1:B:99:TRP:CD1	1.81	0.98
1:B:172:ASP:O	1:B:174:GLU:N	1.95	0.98
1:A:57:LEU:N	1:A:57:LEU:HD13	1.74	0.98
1:B:98:THR:HG23	1:B:221:THR:CA	1.93	0.98
1:A:115:ASN:O	1:A:116:ASN:O	1.81	0.98
1:B:105:SER:HB2	1:B:109:THR:HG22	1.44	0.98
1:B:42:ILE:HG21	1:B:137:LYS:CG	1.94	0.98
1:B:17:VAL:HG21	1:B:67:PRO:HG2	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB2	1:A:109:THR:HG22	1.44	0.97
1:A:146:ASP:HB2	1:A:192:LYS:HZ1	1.27	0.97
1:A:98:THR:HG23	1:A:221:THR:CA	1.93	0.97
1:A:42:ILE:HG21	1:A:137:LYS:CG	1.94	0.97
1:B:80:ARG:CD	1:B:279:PHE:CE1	2.46	0.97
1:B:69:ILE:HG21	1:B:76:LEU:HB3	1.45	0.97
1:A:1:THR:OG1	1:A:32:ILE:CD1	2.13	0.97
1:A:244:VAL:HA	1:A:252:TYR:HD1	1.27	0.97
1:A:36:ALA:O	1:A:37:ASP:HB2	1.64	0.97
1:A:7:ILE:HG21	1:A:16:LYS:N	1.80	0.97
1:B:127:ILE:HG22	1:B:128:ALA:H	1.08	0.97
1:A:122:GLN:NE2	1:A:124:GLY:HA3	1.79	0.96
1:B:163:LEU:HD21	1:B:176:TYR:CD2	1.99	0.96
1:B:123:ILE:HD12	1:B:177:PHE:CD2	1.94	0.96
1:A:123:ILE:HD12	1:A:177:PHE:CD2	1.94	0.96
1:A:13:LEU:HD21	1:A:76:LEU:HD13	1.46	0.96
1:A:105:SER:HB2	1:A:112:VAL:HA	1.44	0.96
1:A:158:ASP:CG	1:A:160:ASN:HD21	1.68	0.96
1:A:53:THR:H	1:A:88:TYR:H	1.09	0.96
1:B:105:SER:HB2	1:B:112:VAL:HA	1.44	0.96
1:B:244:VAL:HA	1:B:252:TYR:HD1	1.27	0.96
1:A:277:LYS:CG	1:B:125:GLU:OE2	2.13	0.96
1:B:134:LYS:HE3	1:B:158:ASP:OD1	1.65	0.96
1:A:139:LEU:HB2	1:A:155:ILE:HG22	1.48	0.96
1:B:163:LEU:HD23	1:B:176:TYR:CD2	1.98	0.96
1:A:5:ARG:HH12	1:A:260:ILE:CB	1.79	0.96
1:A:142:MET:HE2	1:A:202:PHE:CZ	1.97	0.96
1:A:209:LYS:HG3	1:A:213:TYR:CD2	2.00	0.96
1:A:59:ILE:HG22	1:A:66:ASN:C	1.85	0.96
1:A:68:ILE:HG22	1:A:69:ILE:N	1.75	0.96
1:B:209:LYS:HG3	1:B:213:TYR:CD2	2.00	0.96
1:B:51:ARG:CB	1:B:51:ARG:NH1	2.28	0.96
1:A:125:GLU:OE2	1:B:277:LYS:CG	2.13	0.96
1:B:67:PRO:O	1:B:68:ILE:HG12	1.65	0.96
1:B:142:MET:HE2	1:B:202:PHE:CZ	2.01	0.96
1:B:32:ILE:O	1:B:97:GLN:CG	2.14	0.96
1:A:98:THR:CG2	1:A:221:THR:CA	2.44	0.95
1:A:80:ARG:HH11	1:A:279:PHE:HE1	1.14	0.95
1:B:122:GLN:NE2	1:B:124:GLY:HA3	1.79	0.95
1:B:158:ASP:CG	1:B:160:ASN:HD21	1.68	0.95
1:B:83:PHE:CE1	1:B:280:PHE:HE2	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG22	1:B:66:ASN:C	1.85	0.95
1:B:98:THR:CG2	1:B:221:THR:CA	2.44	0.95
1:A:51:ARG:NH1	1:A:51:ARG:CB	2.28	0.95
1:B:192:LYS:CB	1:B:197:LYS:HB2	1.96	0.95
1:B:80:ARG:HH11	1:B:279:PHE:HE1	1.14	0.95
1:A:163:LEU:HD21	1:A:176:TYR:CD2	1.99	0.95
1:A:9:ALA:HB3	1:A:15:TYR:CA	1.96	0.95
1:B:1:THR:OG1	1:B:32:ILE:CD1	2.13	0.95
1:B:13:LEU:HD21	1:B:76:LEU:HD13	1.46	0.95
1:B:146:ASP:HB2	1:B:192:LYS:HZ1	1.27	0.95
1:A:1:THR:H1	1:A:133:VAL:HG11	1.28	0.95
1:A:8:GLY:HA3	1:A:266:LYS:HG3	1.49	0.95
1:B:5:ARG:HH12	1:B:260:ILE:CB	1.79	0.94
1:A:134:LYS:HE3	1:A:158:ASP:OD1	1.65	0.94
1:A:192:LYS:CB	1:A:197:LYS:HB2	1.97	0.94
1:A:98:THR:HG21	1:A:221:THR:OG1	0.77	0.94
1:B:139:LEU:HB2	1:B:155:ILE:HG22	1.48	0.94
1:B:1:THR:HG21	1:B:19:ILE:HD12	0.95	0.94
1:A:110:LYS:C	1:A:112:VAL:H	1.66	0.94
1:A:144:LEU:HG	1:A:151:ASP:HB3	1.46	0.94
1:B:98:THR:HG21	1:B:221:THR:OG1	0.77	0.94
1:A:25:PRO:CG	1:A:257:SER:HB3	1.98	0.94
1:A:67:PRO:O	1:A:68:ILE:HG12	1.66	0.94
1:B:144:LEU:HG	1:B:151:ASP:HB3	1.46	0.94
1:A:32:ILE:O	1:A:97:GLN:CG	2.14	0.94
1:B:271:ILE:HB	1:B:275:ILE:HD11	1.50	0.94
1:B:30:HIS:NE2	1:B:241:LEU:HA	1.83	0.94
1:B:136:VAL:CA	1:B:159:ILE:HG13	1.96	0.93
1:B:225:TRP:HZ3	1:B:226:LYS:HG2	1.25	0.93
1:B:25:PRO:CG	1:B:257:SER:HB3	1.98	0.93
1:B:36:ALA:O	1:B:37:ASP:HB2	1.64	0.93
1:B:19:ILE:HD12	1:B:26:VAL:HG11	1.49	0.93
1:B:50:PRO:O	1:B:53:THR:OG1	1.86	0.93
1:B:13:LEU:CD2	1:B:76:LEU:HD11	1.97	0.93
1:A:136:VAL:CA	1:A:159:ILE:HG13	1.96	0.93
1:A:271:ILE:HB	1:A:275:ILE:HD11	1.50	0.93
1:A:38:LYS:CB	1:A:41:ASN:HB2	1.99	0.93
1:A:50:PRO:O	1:A:53:THR:OG1	1.86	0.93
1:B:7:ILE:HG21	1:B:16:LYS:N	1.80	0.93
1:B:9:ALA:HB3	1:B:15:TYR:CA	1.96	0.93
1:A:13:LEU:CD2	1:A:76:LEU:HD11	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:O	1:B:183:ALA:HB2	1.69	0.93
1:B:190:ILE:CA	1:B:193:ILE:HG12	1.90	0.93
1:B:32:ILE:CG2	1:B:96:PRO:HG2	1.99	0.93
1:A:105:SER:CB	1:A:112:VAL:CA	2.29	0.93
1:A:142:MET:HE2	1:A:202:PHE:CE1	2.01	0.92
1:A:30:HIS:NE2	1:A:241:LEU:HA	1.83	0.92
1:A:5:ARG:HH11	1:A:260:ILE:HG21	1.17	0.92
1:B:105:SER:CB	1:B:112:VAL:CA	2.29	0.92
1:B:188:PHE:O	1:B:191:TYR:HB3	1.69	0.92
1:A:1:THR:HG21	1:A:19:ILE:HD12	0.95	0.92
1:A:38:LYS:O	1:A:41:ASN:N	2.02	0.92
1:B:164:ALA:CB	1:B:165:PRO:CD	2.47	0.92
1:B:38:LYS:O	1:B:41:ASN:N	2.02	0.92
1:A:13:LEU:CD2	1:A:76:LEU:HD13	1.97	0.92
1:A:188:PHE:O	1:A:191:TYR:HB3	1.69	0.92
1:B:82:CYS:SG	1:B:190:ILE:CG1	2.57	0.92
1:A:42:ILE:HB	1:A:137:LYS:HA	1.52	0.92
1:A:89:ILE:O	1:A:90:HIS:HB2	1.69	0.92
1:A:142:MET:CE	1:A:202:PHE:HZ	1.81	0.92
1:B:13:LEU:CD2	1:B:76:LEU:HD13	1.97	0.92
1:B:8:GLY:HA3	1:B:266:LYS:HG3	1.49	0.92
1:B:139:LEU:HB2	1:B:155:ILE:HG21	0.93	0.92
1:A:51:ARG:HB3	1:A:51:ARG:NH1	1.83	0.92
1:A:46:VAL:O	1:A:93:GLY:HA2	1.70	0.92
1:A:97:GLN:HB3	1:A:222:HIS:HD1	1.33	0.92
1:B:42:ILE:HB	1:B:137:LYS:HA	1.52	0.92
1:A:82:CYS:SG	1:A:190:ILE:CG1	2.57	0.92
1:A:83:PHE:CE1	1:A:280:PHE:HE2	1.81	0.92
1:B:29:PHE:HZ	1:B:99:TRP:HD1	1.09	0.92
1:A:225:TRP:HZ3	1:A:226:LYS:HG2	1.25	0.92
1:A:32:ILE:CG2	1:A:96:PRO:HG2	1.99	0.92
1:B:38:LYS:CB	1:B:41:ASN:HB2	1.99	0.92
1:A:190:ILE:O	1:A:194:PRO:HD2	1.70	0.92
1:A:58:GLU:HG3	1:A:70:GLN:HE21	1.29	0.92
1:A:41:ASN:HD21	1:A:137:LYS:HE2	1.36	0.91
1:A:222:HIS:CD2	1:A:226:LYS:HG3	2.05	0.91
1:A:29:PHE:HZ	1:A:99:TRP:HD1	1.09	0.91
1:A:64:THR:C	1:A:65:LEU:HD22	1.91	0.91
1:B:6:GLN:OE1	1:B:265:PRO:HB3	1.70	0.91
1:B:58:GLU:HG3	1:B:70:GLN:HE21	1.29	0.91
1:A:6:GLN:OE1	1:A:265:PRO:HB3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:O	1:B:243:ASN:OD1	1.88	0.91
1:B:53:THR:H	1:B:88:TYR:H	1.09	0.91
1:A:171:GLU:O	1:A:172:ASP:O	1.89	0.91
1:B:64:THR:C	1:B:65:LEU:HD22	1.91	0.91
1:A:139:LEU:HB2	1:A:155:ILE:HG21	0.93	0.91
1:A:242:THR:HA	1:A:251:THR:HB	1.53	0.91
1:B:109:THR:HG23	1:B:150:THR:HG1	1.32	0.91
1:B:190:ILE:O	1:B:194:PRO:HD2	1.70	0.91
1:B:41:ASN:HD21	1:B:137:LYS:HE2	1.36	0.91
1:A:6:GLN:OE1	1:A:265:PRO:CB	2.19	0.91
1:A:80:ARG:HD2	1:A:279:PHE:CD1	2.05	0.91
1:B:222:HIS:CD2	1:B:226:LYS:HG3	2.05	0.91
1:B:242:THR:HA	1:B:251:THR:HB	1.53	0.91
1:A:179:GLY:O	1:A:183:ALA:HB2	1.69	0.91
1:A:42:ILE:HG21	1:A:159:ILE:CD1	2.01	0.91
1:B:46:VAL:O	1:B:93:GLY:HA2	1.69	0.91
1:A:59:ILE:HG22	1:A:67:PRO:CA	2.00	0.91
1:B:123:ILE:HD11	1:B:177:PHE:HE2	1.09	0.91
1:A:164:ALA:CB	1:A:165:PRO:CD	2.47	0.90
1:A:19:ILE:HD12	1:A:26:VAL:HG11	1.49	0.90
1:A:42:ILE:CD1	1:A:159:ILE:HD12	1.96	0.90
1:B:97:GLN:HB3	1:B:222:HIS:HD1	1.33	0.90
1:B:51:ARG:NH1	1:B:51:ARG:HB3	1.82	0.90
1:B:136:VAL:HG11	1:B:156:ALA:HB1	1.53	0.90
1:B:6:GLN:OE1	1:B:265:PRO:CB	2.19	0.90
1:B:80:ARG:HD2	1:B:279:PHE:CD1	2.05	0.90
1:A:123:ILE:HD11	1:A:177:PHE:HE2	1.09	0.90
1:A:190:ILE:CA	1:A:193:ILE:HG12	1.90	0.90
1:B:42:ILE:HG21	1:B:159:ILE:CD1	2.01	0.90
1:A:146:ASP:OD1	1:A:147:GLU:CD	2.10	0.90
1:A:241:LEU:O	1:A:243:ASN:OD1	1.88	0.90
1:B:200:ASN:C	1:B:201:GLN:HG3	1.91	0.90
1:B:163:LEU:HD22	1:B:177:PHE:CZ	2.07	0.90
1:B:25:PRO:HG2	1:B:257:SER:CB	2.02	0.90
1:B:59:ILE:HG22	1:B:67:PRO:CA	2.01	0.90
1:A:56:LYS:C	1:A:57:LEU:HD13	1.92	0.89
1:B:166:LYS:HD3	1:B:176:TYR:HE2	1.37	0.89
1:B:98:THR:CG2	1:B:221:THR:CB	2.39	0.89
1:B:45:MET:HE2	1:B:120:VAL:HG11	1.53	0.89
1:B:171:GLU:O	1:B:172:ASP:O	1.89	0.89
1:B:38:LYS:O	1:B:40:ASP:N	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:C	1:B:57:LEU:HD13	1.92	0.89
1:B:89:ILE:O	1:B:90:HIS:HB2	1.69	0.89
1:A:204:PHE:C	1:A:206:GLY:H	1.76	0.89
1:A:222:HIS:CE1	1:A:226:LYS:HE2	2.07	0.89
1:B:1:THR:H1	1:B:133:VAL:HG11	1.26	0.89
1:B:191:TYR:CE2	1:B:192:LYS:HG3	2.06	0.89
1:A:244:VAL:HB	1:A:254:LYS:HA	1.52	0.89
1:A:25:PRO:HG2	1:A:257:SER:CB	2.02	0.89
1:B:29:PHE:CZ	1:B:99:TRP:CD1	2.59	0.89
1:A:105:SER:H	1:A:112:VAL:HG12	1.38	0.89
1:A:166:LYS:HD3	1:A:176:TYR:HE2	1.37	0.89
1:A:29:PHE:CE1	1:A:225:TRP:HD1	1.91	0.89
1:A:38:LYS:O	1:A:40:ASP:N	2.05	0.89
1:B:244:VAL:HB	1:B:254:LYS:HA	1.52	0.89
1:B:42:ILE:CD1	1:B:159:ILE:HD12	1.95	0.89
1:B:146:ASP:OD1	1:B:147:GLU:CD	2.10	0.89
1:B:158:ASP:O	1:B:160:ASN:N	2.06	0.89
1:B:222:HIS:CE1	1:B:226:LYS:HE2	2.07	0.89
1:B:59:ILE:CG2	1:B:67:PRO:N	2.35	0.89
1:A:127:ILE:HG22	1:A:128:ALA:H	1.08	0.89
1:A:136:VAL:HG11	1:A:156:ALA:HB1	1.53	0.89
1:A:271:ILE:HB	1:A:275:ILE:CD1	2.02	0.89
1:A:144:LEU:HD21	1:A:153:LYS:CD	2.02	0.88
1:A:163:LEU:HD22	1:A:177:PHE:CZ	2.07	0.88
1:A:191:TYR:CE2	1:A:192:LYS:HG3	2.06	0.88
1:B:81:ASN:OD1	1:B:87:GLY:HA2	1.73	0.88
1:A:45:MET:HE1	1:A:120:VAL:CG1	2.03	0.88
1:B:238:GLY:O	1:B:239:ILE:HG23	1.74	0.88
1:A:30:HIS:HE2	1:A:241:LEU:HA	1.38	0.88
1:B:193:ILE:CB	1:B:194:PRO:CD	2.52	0.88
1:B:29:PHE:CE1	1:B:225:TRP:HD1	1.91	0.88
1:B:83:PHE:O	1:B:278:TRP:NE1	2.06	0.88
1:B:204:PHE:C	1:B:206:GLY:H	1.76	0.88
1:A:193:ILE:CB	1:A:194:PRO:CD	2.52	0.88
1:A:81:ASN:OD1	1:A:87:GLY:HA2	1.73	0.88
1:B:71:ASN:O	1:B:72:THR:CB	2.22	0.88
1:B:271:ILE:HB	1:B:275:ILE:CD1	2.02	0.88
1:B:80:ARG:CD	1:B:279:PHE:CD1	2.57	0.88
1:A:230:ALA:HB3	1:A:233:SER:OG	1.72	0.88
1:A:10:LYS:H	1:A:15:TYR:HB2	1.33	0.88
1:B:10:LYS:H	1:B:15:TYR:HB2	1.33	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLY:O	1:A:239:ILE:HG23	1.74	0.88
1:B:95:PHE:HE2	1:B:218:ILE:CD1	1.77	0.88
1:A:51:ARG:CG	1:A:90:HIS:H	1.86	0.87
1:B:30:HIS:HE2	1:B:241:LEU:HA	1.38	0.87
1:A:80:ARG:CD	1:A:279:PHE:CD1	2.57	0.87
1:B:1:THR:OG1	1:B:32:ILE:HD11	1.74	0.87
1:B:54:ASN:O	1:B:79:VAL:N	2.07	0.87
1:B:163:LEU:HD23	1:B:167:LEU:HD11	1.57	0.87
1:B:51:ARG:CG	1:B:90:HIS:H	1.86	0.87
1:A:200:ASN:C	1:A:201:GLN:HG3	1.91	0.87
1:A:54:ASN:O	1:A:79:VAL:N	2.07	0.87
1:B:230:ALA:HB3	1:B:233:SER:OG	1.73	0.87
1:B:29:PHE:HE1	1:B:98:THR:O	1.57	0.87
1:B:51:ARG:HG2	1:B:89:ILE:CA	2.04	0.87
1:A:12:THR:O	1:A:13:LEU:CG	2.22	0.87
1:A:163:LEU:HD23	1:A:167:LEU:HD11	1.57	0.87
1:A:83:PHE:O	1:A:278:TRP:NE1	2.06	0.87
1:B:105:SER:H	1:B:112:VAL:HG12	1.38	0.87
1:B:12:THR:O	1:B:13:LEU:CG	2.22	0.87
1:A:123:ILE:HG12	1:A:123:ILE:O	1.74	0.87
1:A:59:ILE:CG2	1:A:67:PRO:N	2.35	0.87
1:B:42:ILE:HG21	1:B:159:ILE:HD11	1.57	0.87
1:A:158:ASP:O	1:A:160:ASN:N	2.06	0.87
1:B:182:ARG:HD3	1:B:185:ASP:OD2	1.74	0.87
1:B:32:ILE:HG21	1:B:96:PRO:HG2	1.56	0.87
1:A:51:ARG:HG2	1:A:89:ILE:CA	2.04	0.87
1:A:147:GLU:OE1	1:A:192:LYS:NZ	2.08	0.86
1:A:182:ARG:HD3	1:A:185:ASP:OD2	1.74	0.86
1:A:9:ALA:HB3	1:A:15:TYR:CG	2.09	0.86
1:B:25:PRO:HG2	1:B:257:SER:HB3	1.56	0.86
1:A:10:LYS:O	1:A:11:ASN:CG	2.14	0.86
1:A:23:GLY:C	1:A:24:LYS:HG3	1.96	0.86
1:B:9:ALA:HB3	1:B:15:TYR:CG	2.09	0.86
1:B:109:THR:O	1:B:109:THR:HG22	1.75	0.86
1:B:1:THR:CG2	1:B:26:VAL:HG11	2.06	0.86
1:A:1:THR:CG2	1:A:26:VAL:HG11	2.06	0.86
1:A:33:PRO:O	1:A:34:LEU:HG	1.75	0.86
1:A:218:ILE:C	1:A:221:THR:HG22	1.96	0.86
1:A:25:PRO:HG2	1:A:257:SER:HB3	1.56	0.86
1:B:19:ILE:O	1:B:26:VAL:CG1	2.24	0.86
1:A:109:THR:HG22	1:A:109:THR:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HA	1:A:166:LYS:HD2	1.58	0.86
1:A:32:ILE:HG21	1:A:96:PRO:HG2	1.56	0.86
1:B:10:LYS:O	1:B:11:ASN:CG	2.14	0.86
1:A:71:ASN:O	1:A:72:THR:CB	2.22	0.86
1:A:10:LYS:H	1:A:15:TYR:CB	1.88	0.85
1:A:192:LYS:HD3	1:A:197:LYS:CD	2.06	0.85
1:A:1:THR:OG1	1:A:32:ILE:HD11	1.74	0.85
1:A:95:PHE:HE2	1:A:218:ILE:CD1	1.77	0.85
1:B:123:ILE:O	1:B:123:ILE:HG12	1.74	0.85
1:B:163:LEU:HA	1:B:166:LYS:HD2	1.57	0.85
1:B:147:GLU:OE1	1:B:192:LYS:NZ	2.08	0.85
1:B:33:PRO:O	1:B:34:LEU:HG	1.76	0.85
1:B:192:LYS:HD3	1:B:197:LYS:CD	2.06	0.85
1:B:23:GLY:C	1:B:24:LYS:HG3	1.96	0.85
1:B:17:VAL:CG2	1:B:67:PRO:HG2	2.07	0.85
1:A:45:MET:CE	1:A:120:VAL:CG1	2.55	0.85
1:A:17:VAL:CG2	1:A:67:PRO:HG2	2.07	0.85
1:B:56:LYS:HZ3	1:B:70:GLN:HE22	1.23	0.85
1:B:49:ILE:HG13	1:B:92:TYR:HB3	1.58	0.85
1:B:7:ILE:HG23	1:B:7:ILE:O	1.76	0.85
1:B:10:LYS:H	1:B:15:TYR:CB	1.88	0.85
1:A:29:PHE:HE1	1:A:98:THR:O	1.57	0.85
1:B:5:ARG:NH1	1:B:260:ILE:HG22	1.88	0.85
1:B:142:MET:CE	1:B:202:PHE:HZ	1.80	0.84
1:A:19:ILE:O	1:A:26:VAL:CG1	2.24	0.84
1:A:5:ARG:NH1	1:A:260:ILE:HG22	1.88	0.84
1:B:45:MET:CE	1:B:120:VAL:CG1	2.55	0.84
1:B:225:TRP:CE3	1:B:226:LYS:HG2	2.13	0.84
1:B:5:ARG:HB3	1:B:263:ALA:CB	2.05	0.84
1:A:7:ILE:O	1:A:7:ILE:HG23	1.76	0.84
1:B:7:ILE:HG22	1:B:16:LYS:H	1.42	0.84
1:B:19:ILE:HD13	1:B:26:VAL:HG11	0.84	0.84
1:A:94:ALA:HA	1:A:118:ILE:O	1.77	0.84
1:A:57:LEU:HB3	1:A:68:ILE:N	1.93	0.84
1:B:144:LEU:HD21	1:B:153:LYS:CD	2.02	0.84
1:A:214:ALA:O	1:A:217:ILE:HG22	1.77	0.84
1:A:48:GLU:OE2	1:A:93:GLY:O	1.96	0.84
1:B:1:THR:HG22	1:B:19:ILE:HD11	0.84	0.84
1:A:42:ILE:HG21	1:A:159:ILE:HD11	1.57	0.84
1:A:109:THR:HG23	1:A:150:THR:HG1	1.40	0.84
1:B:57:LEU:HB3	1:B:68:ILE:N	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ALA:HA	1:B:118:ILE:O	1.77	0.84
1:A:10:LYS:CG	1:A:268:ASP:OD2	2.26	0.84
1:A:136:VAL:HG13	1:A:156:ALA:HB1	1.60	0.83
1:A:38:LYS:HB3	1:A:41:ASN:HB2	1.59	0.83
1:A:49:ILE:HG13	1:A:92:TYR:HB3	1.58	0.83
1:A:33:PRO:HA	1:A:97:GLN:CD	1.98	0.83
1:A:29:PHE:CE1	1:A:98:THR:O	2.31	0.83
1:B:29:PHE:CE1	1:B:98:THR:O	2.31	0.83
1:B:38:LYS:HB3	1:B:41:ASN:HB2	1.59	0.83
1:B:81:ASN:O	1:B:82:CYS:O	1.95	0.83
1:A:1:THR:HG22	1:A:19:ILE:HD11	0.84	0.83
1:B:214:ALA:O	1:B:217:ILE:HG22	1.77	0.83
1:B:218:ILE:C	1:B:221:THR:HG22	1.96	0.83
1:B:247:PRO:HA	1:B:252:TYR:CD2	2.13	0.83
1:A:19:ILE:HD13	1:A:26:VAL:HG11	0.84	0.83
1:A:69:ILE:HG22	1:A:69:ILE:O	1.78	0.83
1:A:56:LYS:HZ3	1:A:70:GLN:HE22	1.24	0.83
1:B:26:VAL:O	1:B:64:THR:CG2	2.26	0.83
1:A:129:TYR:O	1:A:132:GLN:N	2.11	0.83
1:B:122:GLN:HA	1:B:156:ALA:O	1.79	0.83
1:B:48:GLU:OE2	1:B:93:GLY:O	1.96	0.83
1:A:1:THR:O	1:A:2:TYR:CB	2.27	0.83
1:B:200:ASN:O	1:B:201:GLN:CB	2.27	0.83
1:A:3:THR:O	1:A:20:GLU:N	2.11	0.83
1:A:5:ARG:HB3	1:A:263:ALA:CB	2.05	0.83
1:B:109:THR:O	1:B:109:THR:CG2	2.27	0.83
1:A:225:TRP:CE3	1:A:226:LYS:HG2	2.13	0.82
1:A:247:PRO:HA	1:A:252:TYR:CD2	2.13	0.82
1:B:33:PRO:HA	1:B:97:GLN:CD	1.98	0.82
1:B:7:ILE:HG22	1:B:15:TYR:HA	1.59	0.82
1:B:1:THR:O	1:B:2:TYR:CB	2.27	0.82
1:B:3:THR:O	1:B:20:GLU:N	2.11	0.82
1:B:129:TYR:O	1:B:132:GLN:N	2.11	0.82
1:B:53:THR:N	1:B:88:TYR:H	1.77	0.82
1:A:130:THR:O	1:A:130:THR:CG2	2.27	0.82
1:A:7:ILE:HG22	1:A:15:TYR:HA	1.59	0.82
1:A:29:PHE:CZ	1:A:99:TRP:CD1	2.59	0.82
1:A:81:ASN:OD1	1:A:87:GLY:CA	2.27	0.82
1:B:130:THR:CG2	1:B:130:THR:O	2.27	0.82
1:B:136:VAL:HG13	1:B:156:ALA:HB1	1.60	0.82
1:B:190:ILE:HA	1:B:193:ILE:HD11	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HG23	1:B:269:ALA:HB2	1.61	0.82
1:A:1:THR:OG1	1:A:32:ILE:HD12	1.78	0.82
1:A:57:LEU:N	1:A:57:LEU:CD1	2.43	0.82
1:A:53:THR:N	1:A:88:TYR:H	1.76	0.82
1:A:81:ASN:O	1:A:82:CYS:O	1.95	0.82
1:B:1:THR:OG1	1:B:32:ILE:HD12	1.78	0.82
1:A:12:THR:HG23	1:A:269:ALA:HB2	1.61	0.82
1:B:96:PRO:O	1:B:97:GLN:CB	2.28	0.82
1:A:96:PRO:O	1:A:97:GLN:CB	2.28	0.82
1:A:129:TYR:CD2	1:A:132:GLN:HG3	2.15	0.81
1:A:122:GLN:HA	1:A:156:ALA:O	1.79	0.81
1:B:123:ILE:HG13	1:B:123:ILE:O	1.79	0.81
1:B:81:ASN:OD1	1:B:87:GLY:CA	2.27	0.81
1:A:25:PRO:CD	1:A:257:SER:HB3	2.10	0.81
1:B:10:LYS:CG	1:B:268:ASP:OD2	2.26	0.81
1:B:69:ILE:HG22	1:B:77:ARG:H	1.45	0.81
1:A:182:ARG:HH11	1:A:185:ASP:CB	1.93	0.81
1:B:157:ILE:CG2	1:B:158:ASP:N	2.43	0.81
1:A:109:THR:CG2	1:A:109:THR:O	2.27	0.81
1:B:142:MET:HE2	1:B:202:PHE:CE1	2.09	0.81
1:B:69:ILE:O	1:B:69:ILE:HG22	1.78	0.81
1:A:103:ASN:HA	1:A:112:VAL:HG11	1.63	0.81
1:B:182:ARG:HH11	1:B:185:ASP:CB	1.93	0.81
1:A:125:GLU:OE2	1:B:277:LYS:HG3	1.81	0.81
1:B:5:ARG:NH2	1:B:25:PRO:CB	2.43	0.81
1:A:74:GLY:C	1:A:75:LYS:HG3	2.00	0.81
1:B:45:MET:CE	1:B:120:VAL:HG12	2.11	0.81
1:B:57:LEU:CD1	1:B:57:LEU:N	2.43	0.81
1:A:190:ILE:HA	1:A:193:ILE:HD11	1.61	0.81
1:B:27:SER:CA	1:B:64:THR:CG2	2.42	0.81
1:A:26:VAL:O	1:A:64:THR:CG2	2.26	0.81
1:B:25:PRO:CD	1:B:257:SER:HB3	2.10	0.81
1:A:157:ILE:CG2	1:A:158:ASP:N	2.43	0.81
1:A:7:ILE:HG22	1:A:16:LYS:H	1.42	0.81
1:A:4:THR:HG22	1:A:19:ILE:HG12	1.61	0.81
1:A:31:ASP:O	1:A:32:ILE:HD13	1.81	0.81
1:B:190:ILE:C	1:B:193:ILE:HG12	2.01	0.81
1:B:192:LYS:CB	1:B:197:LYS:CB	2.56	0.80
1:B:4:THR:HG22	1:B:19:ILE:HG12	1.61	0.80
1:B:67:PRO:C	1:B:68:ILE:HG12	2.01	0.80
1:A:166:LYS:HD3	1:A:176:TYR:CE2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:O	1:A:201:GLN:CB	2.27	0.80
1:B:129:TYR:CD2	1:B:132:GLN:HG3	2.15	0.80
1:B:74:GLY:C	1:B:75:LYS:HG3	2.00	0.80
1:A:59:ILE:HA	1:A:66:ASN:O	1.81	0.80
1:B:166:LYS:HD3	1:B:176:TYR:CE2	2.15	0.80
1:B:59:ILE:HA	1:B:66:ASN:O	1.81	0.80
1:B:49:ILE:HD12	1:B:92:TYR:CB	2.11	0.80
1:B:164:ALA:HB3	1:B:165:PRO:HD2	1.64	0.80
1:A:167:LEU:HD21	1:A:177:PHE:CE1	2.17	0.80
1:B:173:VAL:O	1:B:177:PHE:N	2.15	0.80
1:A:173:VAL:O	1:A:177:PHE:N	2.15	0.80
1:A:69:ILE:HG22	1:A:77:ARG:H	1.45	0.80
1:B:130:THR:HG22	1:B:130:THR:O	1.82	0.80
1:B:25:PRO:HD2	1:B:257:SER:HB3	1.62	0.80
1:A:164:ALA:HB3	1:A:165:PRO:HD2	1.64	0.80
1:A:19:ILE:HD11	1:A:26:VAL:HG11	1.60	0.80
1:B:103:ASN:HA	1:B:112:VAL:HG11	1.63	0.80
1:B:182:ARG:HH11	1:B:185:ASP:HB3	1.46	0.80
1:B:26:VAL:CG2	1:B:27:SER:N	2.30	0.80
1:A:182:ARG:NH1	1:A:185:ASP:HB3	1.97	0.80
1:A:190:ILE:C	1:A:193:ILE:HG12	2.01	0.80
1:A:8:GLY:HA2	1:A:266:LYS:H	1.47	0.80
1:B:31:ASP:O	1:B:32:ILE:HD13	1.81	0.80
1:A:155:ILE:O	1:A:155:ILE:CG2	2.31	0.80
1:A:249:THR:O	1:A:251:THR:N	2.14	0.79
1:A:25:PRO:HD2	1:A:257:SER:HB3	1.63	0.79
1:A:45:MET:HE2	1:A:120:VAL:HG11	1.62	0.79
1:A:51:ARG:NH1	1:A:51:ARG:HB2	1.98	0.79
1:A:123:ILE:O	1:A:123:ILE:HG13	1.79	0.79
1:A:49:ILE:HD12	1:A:92:TYR:CB	2.11	0.79
1:A:5:ARG:NH2	1:A:25:PRO:CB	2.43	0.79
1:A:93:GLY:O	1:A:94:ALA:HB2	1.82	0.79
1:A:130:THR:HG22	1:A:130:THR:O	1.82	0.79
1:A:277:LYS:HG3	1:B:125:GLU:OE2	1.81	0.79
1:B:167:LEU:HD21	1:B:177:PHE:CE1	2.17	0.79
1:B:182:ARG:NH1	1:B:185:ASP:HB3	1.97	0.79
1:A:217:ILE:O	1:A:220:GLU:OE1	2.01	0.79
1:B:56:LYS:HZ3	1:B:70:GLN:NE2	1.80	0.79
1:B:27:SER:HB2	1:B:64:THR:CG2	2.13	0.79
1:A:152:TRP:O	1:A:153:LYS:HD2	1.82	0.79
1:A:67:PRO:C	1:A:68:ILE:HG12	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:O	1:A:90:HIS:CB	2.29	0.79
1:B:8:GLY:HA2	1:B:266:LYS:H	1.47	0.79
1:A:98:THR:CG2	1:A:221:THR:CB	2.39	0.79
1:B:191:TYR:HE2	1:B:192:LYS:CG	1.95	0.79
1:B:217:ILE:O	1:B:220:GLU:OE1	2.01	0.79
1:B:155:ILE:CG2	1:B:155:ILE:O	2.30	0.79
1:B:152:TRP:O	1:B:153:LYS:HD2	1.82	0.78
1:B:166:LYS:CD	1:B:176:TYR:HE2	1.96	0.78
1:A:164:ALA:CB	1:A:165:PRO:HD3	2.09	0.78
1:B:225:TRP:CZ3	1:B:229:ILE:HD11	2.18	0.78
1:B:249:THR:O	1:B:251:THR:N	2.14	0.78
1:B:68:ILE:CG2	1:B:69:ILE:H	1.95	0.78
1:A:83:PHE:C	1:A:83:PHE:HD2	1.87	0.78
1:B:9:ALA:HB3	1:B:15:TYR:HB2	0.81	0.78
1:B:1:THR:HG23	1:B:26:VAL:HG21	1.65	0.78
1:A:174:GLU:O	1:A:178:PRO:CG	2.32	0.78
1:A:166:LYS:CD	1:A:176:TYR:HE2	1.96	0.78
1:A:225:TRP:CZ3	1:A:229:ILE:HD11	2.18	0.78
1:B:174:GLU:O	1:B:178:PRO:CG	2.32	0.78
1:B:51:ARG:HB2	1:B:51:ARG:NH1	1.98	0.78
1:B:89:ILE:O	1:B:90:HIS:CB	2.29	0.78
1:A:83:PHE:CD2	1:A:83:PHE:C	2.55	0.78
1:B:83:PHE:HD2	1:B:83:PHE:C	1.87	0.78
1:B:102:PRO:O	1:B:112:VAL:HB	1.84	0.78
1:A:28:ALA:HB3	1:A:59:ILE:HD12	1.64	0.78
1:B:191:TYR:CD2	1:B:192:LYS:CG	2.65	0.77
1:A:192:LYS:CB	1:A:197:LYS:CB	2.56	0.77
1:A:7:ILE:HG21	1:A:14:GLU:O	1.85	0.77
1:A:1:THR:HG23	1:A:26:VAL:HG21	1.65	0.77
1:B:142:MET:CB	1:B:153:LYS:CB	2.62	0.77
1:B:1:THR:HG22	1:B:19:ILE:CD1	1.75	0.77
1:A:45:MET:CE	1:A:120:VAL:HG12	2.11	0.77
1:A:146:ASP:HB2	1:A:192:LYS:NZ	1.99	0.77
1:A:191:TYR:CD2	1:A:192:LYS:CG	2.66	0.77
1:A:91:ASN:O	1:A:92:TYR:CB	2.32	0.77
1:A:8:GLY:O	1:A:9:ALA:HB2	1.84	0.77
1:B:161:ASP:OD1	1:B:162:PRO:HD2	1.84	0.77
1:B:35:TYR:H	1:B:35:TYR:HD2	1.32	0.77
1:A:191:TYR:HE2	1:A:192:LYS:CG	1.95	0.77
1:B:83:PHE:CD2	1:B:83:PHE:C	2.55	0.77
1:A:102:PRO:O	1:A:112:VAL:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:NE2	1:A:124:GLY:CA	2.48	0.77
1:B:7:ILE:HG21	1:B:14:GLU:O	1.85	0.77
1:B:244:VAL:HB	1:B:254:LYS:CA	2.15	0.77
1:B:54:ASN:HB3	1:B:79:VAL:O	1.84	0.77
1:B:93:GLY:O	1:B:94:ALA:HB2	1.82	0.77
1:A:161:ASP:OD1	1:A:162:PRO:HD2	1.84	0.77
1:B:122:GLN:NE2	1:B:124:GLY:CA	2.48	0.77
1:B:246:LEU:C	1:B:248:ASP:H	1.88	0.77
1:A:56:LYS:HZ3	1:A:70:GLN:NE2	1.82	0.77
1:B:192:LYS:HB3	1:B:197:LYS:HB3	1.65	0.76
1:A:83:PHE:CD1	1:A:280:PHE:CZ	2.74	0.76
1:B:48:GLU:C	1:B:49:ILE:HG12	2.06	0.76
1:B:53:THR:H	1:B:88:TYR:N	1.83	0.76
1:A:94:ALA:O	1:A:96:PRO:N	2.18	0.76
1:B:83:PHE:CD1	1:B:280:PHE:CZ	2.74	0.76
1:B:2:TYR:HB2	1:B:21:LYS:HA	1.68	0.76
1:A:35:TYR:H	1:A:35:TYR:HD2	1.32	0.76
1:A:27:SER:CA	1:A:64:THR:CG2	2.42	0.76
1:B:114:ASP:HB3	1:B:149:GLU:OE1	1.85	0.76
1:B:193:ILE:N	1:B:197:LYS:O	2.19	0.76
1:B:28:ALA:HB3	1:B:59:ILE:HD12	1.64	0.76
1:A:193:ILE:N	1:A:197:LYS:O	2.19	0.76
1:A:95:PHE:CD2	1:A:218:ILE:CD1	2.65	0.76
1:A:68:ILE:CG2	1:A:69:ILE:H	1.95	0.76
1:A:83:PHE:HA	1:A:278:TRP:CD1	2.20	0.76
1:B:122:GLN:CB	1:B:156:ALA:O	2.34	0.76
1:B:83:PHE:HA	1:B:278:TRP:CD1	2.20	0.76
1:A:48:GLU:C	1:A:49:ILE:HG12	2.06	0.76
1:A:114:ASP:HB3	1:A:149:GLU:OE1	1.85	0.76
1:A:54:ASN:HB3	1:A:79:VAL:O	1.84	0.76
1:A:97:GLN:O	1:A:225:TRP:CD2	2.39	0.76
1:B:146:ASP:HB2	1:B:192:LYS:NZ	1.99	0.76
1:B:118:ILE:HD12	1:B:221:THR:OG1	1.86	0.76
1:B:44:ASN:OD1	1:B:44:ASN:N	2.18	0.76
1:A:182:ARG:HH11	1:A:185:ASP:HB3	1.46	0.76
1:B:19:ILE:HD11	1:B:26:VAL:HG11	1.60	0.76
1:B:94:ALA:O	1:B:96:PRO:N	2.18	0.76
1:B:147:GLU:CD	1:B:192:LYS:HZ3	1.89	0.75
1:B:98:THR:HA	1:B:225:TRP:HB3	1.68	0.75
1:A:1:THR:HG22	1:A:19:ILE:CD1	1.75	0.75
1:B:80:ARG:HD2	1:B:279:PHE:HE1	1.47	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:CB	1:A:153:LYS:CB	2.62	0.75
1:A:1:THR:CB	1:A:19:ILE:HD11	2.12	0.75
1:A:53:THR:H	1:A:88:TYR:N	1.83	0.75
1:B:32:ILE:HG21	1:B:96:PRO:CG	2.17	0.75
1:A:9:ALA:HB3	1:A:15:TYR:HB2	0.81	0.75
1:B:24:LYS:HB3	1:B:25:PRO:HD2	1.68	0.75
1:A:44:ASN:N	1:A:44:ASN:OD1	2.18	0.75
1:A:244:VAL:HB	1:A:254:LYS:CA	2.15	0.75
1:A:32:ILE:HG21	1:A:96:PRO:CG	2.17	0.75
1:B:137:LYS:HG3	1:B:159:ILE:CG1	2.16	0.75
1:B:8:GLY:O	1:B:9:ALA:HB2	1.84	0.75
1:A:192:LYS:HB3	1:A:197:LYS:HB3	1.65	0.75
1:B:1:THR:HG21	1:B:26:VAL:HG11	1.67	0.75
1:B:97:GLN:O	1:B:225:TRP:CD2	2.39	0.75
1:A:139:LEU:HD12	1:A:155:ILE:CG2	2.17	0.75
1:B:19:ILE:O	1:B:26:VAL:HG13	1.86	0.75
1:A:277:LYS:CD	1:B:125:GLU:OE2	2.35	0.74
1:B:142:MET:HB3	1:B:153:LYS:CB	2.17	0.74
1:B:38:LYS:HB3	1:B:41:ASN:CB	2.17	0.74
1:B:6:GLN:HG2	1:B:15:TYR:HE1	1.51	0.74
1:A:137:LYS:HG3	1:A:159:ILE:CG1	2.16	0.74
1:A:122:GLN:CB	1:A:156:ALA:O	2.34	0.74
1:A:98:THR:HA	1:A:225:TRP:HB3	1.68	0.74
1:A:36:ALA:O	1:A:37:ASP:CB	2.34	0.74
1:B:101:ASP:OD1	1:B:102:PRO:HD2	1.87	0.74
1:A:27:SER:HB2	1:A:64:THR:CG2	2.13	0.74
1:A:45:MET:CE	1:A:120:VAL:HG11	2.17	0.74
1:B:164:ALA:CB	1:B:165:PRO:HD3	2.09	0.74
1:B:1:THR:O	1:B:21:LYS:HA	1.87	0.74
1:B:80:ARG:HG3	1:B:194:PRO:CB	2.18	0.74
1:A:177:PHE:N	1:A:177:PHE:CD1	2.56	0.74
1:A:38:LYS:HB3	1:A:41:ASN:CB	2.17	0.74
1:A:28:ALA:O	1:A:65:LEU:HD23	1.87	0.74
1:B:28:ALA:O	1:B:65:LEU:HD23	1.87	0.74
1:A:24:LYS:HB3	1:A:25:PRO:HD2	1.68	0.74
1:B:95:PHE:CD2	1:B:218:ILE:CD1	2.65	0.74
1:B:84:PRO:O	1:B:85:HIS:CB	2.35	0.74
1:A:157:ILE:HG22	1:A:158:ASP:N	2.02	0.74
1:A:5:ARG:HH22	1:A:25:PRO:HB3	1.52	0.74
1:A:6:GLN:HG2	1:A:15:TYR:HE1	1.51	0.74
1:A:69:ILE:HB	1:A:76:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:OE2	1:B:277:LYS:CD	2.35	0.73
1:B:176:TYR:HB3	1:B:177:PHE:CE1	2.23	0.73
1:A:1:THR:O	1:A:21:LYS:HA	1.88	0.73
1:A:118:ILE:HD12	1:A:221:THR:OG1	1.86	0.73
1:A:101:ASP:OD1	1:A:102:PRO:HD2	1.87	0.73
1:A:147:GLU:CD	1:A:192:LYS:HZ3	1.91	0.73
1:A:95:PHE:HE2	1:A:218:ILE:HD11	0.92	0.73
1:A:97:GLN:HB3	1:A:222:HIS:ND1	2.04	0.73
1:B:146:ASP:CB	1:B:192:LYS:HZ1	2.01	0.73
1:B:57:LEU:CB	1:B:68:ILE:O	2.35	0.73
1:A:144:LEU:N	1:A:144:LEU:HD23	2.03	0.73
1:A:2:TYR:HB2	1:A:21:LYS:HA	1.68	0.73
1:A:80:ARG:HG3	1:A:194:PRO:CB	2.18	0.73
1:B:38:LYS:HG2	1:B:41:ASN:CB	2.17	0.73
1:A:19:ILE:O	1:A:26:VAL:HG13	1.86	0.73
1:B:84:PRO:C	1:B:85:HIS:CG	2.61	0.73
1:B:93:GLY:O	1:B:94:ALA:CB	2.37	0.73
1:B:45:MET:CE	1:B:120:VAL:HG11	2.17	0.73
1:B:139:LEU:HD12	1:B:155:ILE:CG2	2.17	0.73
1:A:176:TYR:HB3	1:A:177:PHE:CE1	2.23	0.73
1:A:57:LEU:CB	1:A:68:ILE:O	2.35	0.73
1:A:84:PRO:O	1:A:85:HIS:CB	2.35	0.73
1:B:244:VAL:CB	1:B:254:LYS:HA	2.18	0.73
1:B:91:ASN:O	1:B:92:TYR:CB	2.32	0.73
1:A:47:VAL:HG21	1:A:129:TYR:H	1.53	0.72
1:A:93:GLY:O	1:A:94:ALA:CB	2.37	0.72
1:B:144:LEU:N	1:B:144:LEU:HD23	2.03	0.72
1:B:157:ILE:HG22	1:B:158:ASP:N	2.02	0.72
1:A:10:LYS:N	1:A:15:TYR:HB2	2.04	0.72
1:A:60:THR:HA	1:A:65:LEU:HD12	1.71	0.72
1:B:177:PHE:N	1:B:177:PHE:CD1	2.56	0.72
1:B:69:ILE:HB	1:B:76:LEU:HD12	1.69	0.72
1:A:38:LYS:HG2	1:A:41:ASN:CB	2.16	0.72
1:A:1:THR:HG21	1:A:26:VAL:HG11	1.67	0.72
1:A:84:PRO:C	1:A:85:HIS:CG	2.61	0.72
1:B:1:THR:HB	1:B:133:VAL:HG21	1.71	0.72
1:A:129:TYR:CD2	1:A:132:GLN:CG	2.72	0.72
1:A:246:LEU:C	1:A:248:ASP:H	1.89	0.72
1:B:47:VAL:HG21	1:B:129:TYR:H	1.53	0.72
1:B:1:THR:CB	1:B:19:ILE:HD11	2.12	0.72
1:A:105:SER:HB3	1:A:112:VAL:HA	0.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:THR:HB	1:A:133:VAL:HG21	1.71	0.72
1:A:82:CYS:HG	1:A:190:ILE:HG13	1.52	0.72
1:A:4:THR:HB	1:A:19:ILE:CA	2.13	0.72
1:B:129:TYR:O	1:B:130:THR:C	2.28	0.72
1:A:191:TYR:HD2	1:A:192:LYS:HG3	1.55	0.72
1:B:19:ILE:O	1:B:26:VAL:HG12	1.90	0.72
1:B:4:THR:HB	1:B:19:ILE:CA	2.13	0.72
1:B:51:ARG:C	1:B:88:TYR:O	2.28	0.72
1:A:253:SER:C	1:A:255:ALA:H	1.92	0.72
1:A:69:ILE:O	1:A:70:GLN:C	2.28	0.71
1:B:60:THR:HA	1:B:65:LEU:HD12	1.71	0.71
1:B:253:SER:C	1:B:255:ALA:H	1.92	0.71
1:B:97:GLN:HB3	1:B:222:HIS:ND1	2.04	0.71
1:A:25:PRO:CG	1:A:257:SER:CB	2.65	0.71
1:A:49:ILE:CD1	1:A:92:TYR:CG	2.50	0.71
1:A:41:ASN:ND2	1:A:137:LYS:HE2	2.05	0.71
1:B:29:PHE:H	1:B:96:PRO:HB2	1.56	0.71
1:A:272:ASP:O	1:A:275:ILE:HG13	1.91	0.71
1:B:5:ARG:HH22	1:B:25:PRO:HB3	1.52	0.71
1:A:142:MET:HB3	1:A:153:LYS:CB	2.17	0.71
1:A:56:LYS:C	1:A:57:LEU:CD1	2.59	0.71
1:B:69:ILE:O	1:B:70:GLN:C	2.28	0.71
1:A:158:ASP:CB	1:A:160:ASN:HD21	2.04	0.71
1:A:244:VAL:CB	1:A:254:LYS:HA	2.18	0.71
1:B:129:TYR:CD2	1:B:132:GLN:CG	2.72	0.71
1:A:105:SER:HB3	1:A:112:VAL:CG1	2.21	0.71
1:A:29:PHE:CE1	1:A:225:TRP:CD1	2.78	0.71
1:A:51:ARG:C	1:A:88:TYR:O	2.28	0.71
1:B:4:THR:HG22	1:B:19:ILE:CG1	2.21	0.71
1:B:232:LYS:O	1:B:233:SER:C	2.29	0.71
1:A:11:ASN:O	1:A:12:THR:C	2.29	0.71
1:A:1:THR:H3	1:A:133:VAL:HG11	1.54	0.71
1:B:27:SER:HA	1:B:64:THR:HG22	1.71	0.71
1:B:7:ILE:O	1:B:8:GLY:C	2.29	0.71
1:A:105:SER:HB3	1:A:112:VAL:CB	2.21	0.70
1:B:158:ASP:CB	1:B:160:ASN:HD21	2.04	0.70
1:B:56:LYS:C	1:B:57:LEU:CD1	2.59	0.70
1:A:129:TYR:O	1:A:130:THR:C	2.28	0.70
1:A:28:ALA:CB	1:A:59:ILE:HD12	2.21	0.70
1:B:41:ASN:ND2	1:B:137:LYS:HE2	2.05	0.70
1:B:42:ILE:CG2	1:B:159:ILE:HD11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:HB3	1:B:161:ASP:HB3	1.74	0.70
1:B:191:TYR:HD2	1:B:192:LYS:HG3	1.55	0.70
1:A:146:ASP:CB	1:A:192:LYS:HZ1	2.02	0.70
1:A:174:GLU:C	1:A:178:PRO:HB3	2.05	0.70
1:B:249:THR:C	1:B:251:THR:H	1.94	0.70
1:B:25:PRO:CG	1:B:257:SER:CB	2.65	0.70
1:B:49:ILE:CD1	1:B:92:TYR:CB	2.69	0.70
1:A:192:LYS:NZ	1:A:200:ASN:HD21	1.90	0.70
1:B:242:THR:O	1:B:243:ASN:OD1	2.09	0.70
1:B:36:ALA:O	1:B:37:ASP:CB	2.34	0.70
1:A:122:GLN:CA	1:A:156:ALA:O	2.40	0.70
1:A:49:ILE:CD1	1:A:92:TYR:CB	2.69	0.70
1:A:42:ILE:CG2	1:A:159:ILE:HD11	2.21	0.70
1:A:158:ASP:HB3	1:A:161:ASP:HB3	1.74	0.70
1:A:45:MET:SD	1:A:93:GLY:HA3	2.31	0.70
1:A:7:ILE:O	1:A:8:GLY:C	2.29	0.70
1:A:29:PHE:H	1:A:96:PRO:HB2	1.56	0.70
1:B:122:GLN:CA	1:B:156:ALA:O	2.40	0.70
1:A:81:ASN:O	1:A:82:CYS:C	2.30	0.70
1:A:242:THR:O	1:A:243:ASN:OD1	2.09	0.70
1:A:28:ALA:O	1:A:29:PHE:HB3	1.91	0.70
1:B:45:MET:SD	1:B:93:GLY:HA3	2.31	0.70
1:A:112:VAL:O	1:A:150:THR:OG1	2.10	0.69
1:A:4:THR:HG22	1:A:19:ILE:CG1	2.21	0.69
1:B:28:ALA:CB	1:B:59:ILE:HD12	2.21	0.69
1:B:94:ALA:O	1:B:96:PRO:HD3	1.92	0.69
1:A:47:VAL:HG22	1:A:131:GLY:H	1.57	0.69
1:A:232:LYS:O	1:A:233:SER:C	2.29	0.69
1:B:105:SER:HB3	1:B:112:VAL:CG1	2.21	0.69
1:B:105:SER:HB3	1:B:112:VAL:HA	0.72	0.69
1:B:11:ASN:O	1:B:12:THR:C	2.29	0.69
1:B:95:PHE:HE2	1:B:218:ILE:HD11	0.93	0.69
1:B:105:SER:HB3	1:B:112:VAL:CB	2.21	0.69
1:B:84:PRO:O	1:B:85:HIS:CD2	2.45	0.69
1:A:141:ILE:HA	1:A:153:LYS:O	1.92	0.69
1:B:192:LYS:NZ	1:B:200:ASN:HD21	1.90	0.69
1:B:272:ASP:O	1:B:275:ILE:HG13	1.91	0.69
1:B:49:ILE:CD1	1:B:92:TYR:CG	2.50	0.69
1:B:1:THR:H3	1:B:133:VAL:HG11	1.56	0.69
1:A:84:PRO:O	1:A:85:HIS:CD2	2.46	0.69
1:B:4:THR:CG2	1:B:19:ILE:HA	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:HA	1:B:153:LYS:O	1.92	0.69
1:B:28:ALA:O	1:B:29:PHE:HB3	1.91	0.69
1:A:249:THR:C	1:A:251:THR:H	1.95	0.69
1:B:29:PHE:CE1	1:B:225:TRP:CD1	2.78	0.69
1:B:209:LYS:HG3	1:B:213:TYR:CG	2.28	0.69
1:B:158:ASP:CB	1:B:160:ASN:ND2	2.56	0.69
1:B:58:GLU:O	1:B:59:ILE:HG22	1.93	0.69
1:B:56:LYS:NZ	1:B:70:GLN:CD	2.46	0.69
1:A:105:SER:HB2	1:A:109:THR:CG2	2.20	0.69
1:A:158:ASP:CB	1:A:160:ASN:ND2	2.56	0.69
1:B:112:VAL:O	1:B:150:THR:OG1	2.10	0.69
1:A:102:PRO:HA	1:A:113:GLY:O	1.93	0.68
1:A:19:ILE:O	1:A:26:VAL:HG12	1.90	0.68
1:A:278:TRP:HH2	1:B:89:ILE:HG13	1.56	0.68
1:B:10:LYS:N	1:B:15:TYR:HB2	2.04	0.68
1:B:81:ASN:O	1:B:82:CYS:C	2.30	0.68
1:A:42:ILE:HG22	1:A:137:LYS:HG2	1.72	0.68
1:A:56:LYS:NZ	1:A:70:GLN:CD	2.46	0.68
1:B:47:VAL:HG22	1:B:131:GLY:H	1.57	0.68
1:B:150:THR:HG22	1:B:150:THR:O	1.94	0.68
1:B:8:GLY:CA	1:B:266:LYS:H	2.05	0.68
1:A:4:THR:CG2	1:A:19:ILE:HA	2.22	0.68
1:A:59:ILE:CG1	1:A:59:ILE:O	2.41	0.68
1:B:102:PRO:HA	1:B:113:GLY:O	1.93	0.68
1:B:105:SER:HB2	1:B:109:THR:CG2	2.20	0.68
1:B:143:ALA:O	1:B:202:PHE:CD1	2.47	0.68
1:B:217:ILE:CG2	1:B:218:ILE:N	2.56	0.68
1:A:209:LYS:HG3	1:A:213:TYR:CG	2.28	0.68
1:B:162:PRO:O	1:B:163:LEU:HB2	1.93	0.68
1:B:59:ILE:O	1:B:59:ILE:CG1	2.41	0.68
1:B:49:ILE:CG1	1:B:92:TYR:HB3	2.24	0.68
1:B:97:GLN:O	1:B:225:TRP:CG	2.47	0.68
1:B:103:ASN:O	1:B:104:VAL:CB	2.28	0.68
1:B:174:GLU:C	1:B:178:PRO:HB3	2.05	0.68
1:B:275:ILE:O	1:B:277:LYS:HB2	1.93	0.68
1:A:58:GLU:O	1:A:59:ILE:HG22	1.93	0.68
1:B:23:GLY:O	1:B:24:LYS:CB	2.42	0.68
1:A:162:PRO:O	1:A:163:LEU:HB2	1.93	0.68
1:A:83:PHE:HB3	1:A:84:PRO:HD3	1.75	0.68
1:A:8:GLY:CA	1:A:266:LYS:H	2.05	0.68
1:B:83:PHE:HB3	1:B:84:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:O	1:A:116:ASN:C	2.32	0.68
1:A:191:TYR:HE2	1:A:192:LYS:CE	2.07	0.68
1:A:49:ILE:CG1	1:A:92:TYR:HB3	2.24	0.68
1:A:94:ALA:O	1:A:96:PRO:HD3	1.92	0.68
1:B:92:TYR:CE2	1:B:121:LEU:HD21	2.29	0.68
1:A:122:GLN:HE22	1:A:124:GLY:HA3	1.58	0.68
1:A:12:THR:O	1:A:13:LEU:CB	2.42	0.68
1:A:146:ASP:OD1	1:A:147:GLU:OE2	2.12	0.68
1:A:97:GLN:O	1:A:225:TRP:CG	2.47	0.68
1:B:92:TYR:HD2	1:B:121:LEU:HD23	1.58	0.68
1:B:12:THR:O	1:B:13:LEU:CB	2.42	0.68
1:B:90:HIS:O	1:B:91:ASN:CB	2.41	0.68
1:A:92:TYR:CE2	1:A:121:LEU:HD21	2.29	0.67
1:A:89:ILE:HG13	1:B:278:TRP:HH2	1.57	0.67
1:B:81:ASN:HD22	1:B:276:ASP:HA	1.59	0.67
1:A:241:LEU:O	1:A:242:THR:C	2.32	0.67
1:A:168:ASN:C	1:A:168:ASN:ND2	2.48	0.67
1:A:7:ILE:HG22	1:A:16:LYS:N	2.04	0.67
1:B:42:ILE:HG21	1:B:159:ILE:HD13	1.75	0.67
1:B:241:LEU:O	1:B:242:THR:C	2.32	0.67
1:A:139:LEU:HD12	1:A:155:ILE:HG23	1.76	0.67
1:B:191:TYR:HE2	1:B:192:LYS:CE	2.07	0.67
1:B:247:PRO:HB3	1:B:252:TYR:CE2	2.30	0.67
1:A:143:ALA:O	1:A:202:PHE:CD1	2.47	0.67
1:B:3:THR:O	1:B:20:GLU:O	2.12	0.67
1:A:217:ILE:CG2	1:A:218:ILE:N	2.56	0.67
1:A:23:GLY:O	1:A:24:LYS:CB	2.42	0.67
1:A:247:PRO:HB3	1:A:252:TYR:CE2	2.30	0.67
1:B:123:ILE:HD12	1:B:177:PHE:HD2	1.57	0.67
1:B:168:ASN:ND2	1:B:168:ASN:C	2.48	0.67
1:A:147:GLU:CD	1:A:192:LYS:NZ	2.48	0.67
1:A:28:ALA:HA	1:A:32:ILE:HG12	1.75	0.67
1:B:115:ASN:O	1:B:116:ASN:C	2.32	0.67
1:B:94:ALA:O	1:B:96:PRO:CD	2.42	0.67
1:A:150:THR:HG22	1:A:150:THR:O	1.94	0.67
1:A:42:ILE:HG21	1:A:159:ILE:HD13	1.75	0.67
1:A:275:ILE:O	1:A:277:LYS:HB2	1.93	0.67
1:B:229:ILE:O	1:B:230:ALA:C	2.31	0.67
1:B:83:PHE:HB3	1:B:84:PRO:CD	2.25	0.67
1:A:229:ILE:O	1:A:230:ALA:C	2.31	0.67
1:A:48:GLU:C	1:A:49:ILE:CG1	2.62	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ALA:HA	1:B:32:ILE:HG12	1.75	0.67
1:A:246:LEU:O	1:A:248:ASP:N	2.28	0.67
1:A:25:PRO:CG	1:A:257:SER:CA	2.73	0.66
1:A:83:PHE:HB3	1:A:84:PRO:CD	2.25	0.66
1:A:92:TYR:HD2	1:A:121:LEU:HD23	1.58	0.66
1:B:34:LEU:O	1:B:36:ALA:N	2.24	0.66
1:B:50:PRO:HA	1:B:128:ALA:HB2	1.77	0.66
1:A:56:LYS:HZ2	1:A:70:GLN:CD	1.97	0.66
1:B:146:ASP:OD1	1:B:147:GLU:OE2	2.12	0.66
1:B:93:GLY:N	1:B:120:VAL:O	2.28	0.66
1:A:80:ARG:HD2	1:A:279:PHE:HE1	1.47	0.66
1:B:139:LEU:HD12	1:B:155:ILE:HG23	1.76	0.66
1:A:152:TRP:C	1:A:153:LYS:HD2	2.15	0.66
1:A:94:ALA:O	1:A:96:PRO:CD	2.42	0.66
1:B:141:ILE:CG2	1:B:141:ILE:O	2.43	0.66
1:B:152:TRP:C	1:B:153:LYS:HD2	2.15	0.66
1:B:163:LEU:HD22	1:B:177:PHE:HZ	1.60	0.66
1:A:123:ILE:HD12	1:A:177:PHE:HD2	1.57	0.66
1:A:3:THR:O	1:A:20:GLU:O	2.12	0.66
1:B:25:PRO:HG2	1:B:257:SER:CA	2.25	0.66
1:B:48:GLU:C	1:B:49:ILE:CG1	2.62	0.66
1:B:59:ILE:HB	1:B:66:ASN:N	2.10	0.66
1:A:105:SER:HB2	1:A:109:THR:O	1.95	0.66
1:B:42:ILE:HG22	1:B:137:LYS:HG2	1.72	0.66
1:A:142:MET:CA	1:A:153:LYS:HB2	2.25	0.66
1:B:30:HIS:CD2	1:B:241:LEU:HA	2.31	0.66
1:A:163:LEU:HD23	1:A:167:LEU:CD1	2.25	0.66
1:A:59:ILE:HB	1:A:66:ASN:N	2.10	0.66
1:B:25:PRO:CG	1:B:257:SER:CA	2.73	0.66
1:B:246:LEU:O	1:B:248:ASP:N	2.28	0.66
1:A:93:GLY:N	1:A:120:VAL:O	2.28	0.66
1:A:50:PRO:HA	1:A:128:ALA:HB2	1.78	0.66
1:A:141:ILE:O	1:A:141:ILE:HG22	1.95	0.66
1:A:42:ILE:CG1	1:A:159:ILE:HD11	2.25	0.66
1:B:142:MET:CA	1:B:153:LYS:HB2	2.25	0.66
1:B:163:LEU:HD23	1:B:167:LEU:CD1	2.25	0.66
1:A:25:PRO:HG2	1:A:257:SER:CA	2.25	0.65
1:A:81:ASN:HD22	1:A:276:ASP:HA	1.59	0.65
1:A:27:SER:HA	1:A:64:THR:HG22	1.72	0.65
1:B:141:ILE:HG22	1:B:141:ILE:O	1.95	0.65
1:B:244:VAL:O	1:B:244:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:CG1	1:B:159:ILE:HD11	2.25	0.65
1:B:158:ASP:HB3	1:B:160:ASN:ND2	2.12	0.65
1:B:147:GLU:CD	1:B:192:LYS:NZ	2.48	0.65
1:B:190:ILE:CB	1:B:193:ILE:HG13	2.26	0.65
1:A:34:LEU:O	1:A:36:ALA:N	2.24	0.65
1:B:105:SER:HB2	1:B:109:THR:O	1.96	0.65
1:B:1:THR:O	1:B:2:TYR:CD1	2.50	0.65
1:A:158:ASP:HB3	1:A:160:ASN:ND2	2.12	0.65
1:A:1:THR:O	1:A:2:TYR:CD1	2.50	0.65
1:B:58:GLU:C	1:B:59:ILE:HG23	2.16	0.65
1:A:143:ALA:HA	1:A:152:TRP:HA	1.78	0.65
1:A:163:LEU:CD2	1:A:167:LEU:HD11	2.27	0.65
1:B:114:ASP:CB	1:B:149:GLU:OE1	2.45	0.65
1:B:166:LYS:HB3	1:B:176:TYR:CE2	2.32	0.65
1:B:7:ILE:HG22	1:B:16:LYS:N	2.04	0.65
1:B:7:ILE:O	1:B:15:TYR:HA	1.96	0.65
1:B:190:ILE:CA	1:B:193:ILE:HD11	2.27	0.65
1:B:220:GLU:HG2	1:B:220:GLU:O	1.96	0.65
1:B:46:VAL:O	1:B:93:GLY:CA	2.44	0.65
1:B:53:THR:O	1:B:88:TYR:CB	2.26	0.65
1:B:253:SER:O	1:B:255:ALA:N	2.30	0.65
1:A:106:HIS:CB	1:A:107:PRO:HD2	2.27	0.65
1:A:190:ILE:CB	1:A:193:ILE:HG13	2.26	0.64
1:A:80:ARG:CG	1:A:194:PRO:HB2	2.25	0.64
1:A:1:THR:CG2	1:A:26:VAL:HG21	2.27	0.64
1:A:30:HIS:CD2	1:A:241:LEU:HA	2.31	0.64
1:B:243:ASN:O	1:B:252:TYR:HA	1.97	0.64
1:B:45:MET:HE1	1:B:120:VAL:CG1	2.12	0.64
1:B:139:LEU:O	1:B:211:LYS:CA	2.45	0.64
1:B:106:HIS:CB	1:B:107:PRO:HD2	2.27	0.64
1:A:163:LEU:HA	1:A:166:LYS:CD	2.28	0.64
1:A:17:VAL:O	1:A:66:ASN:HB3	1.97	0.64
1:A:193:ILE:O	1:A:195:ASP:N	2.30	0.64
1:A:7:ILE:O	1:A:15:TYR:HA	1.96	0.64
1:A:173:VAL:HG13	1:A:177:PHE:HB2	1.79	0.64
1:B:17:VAL:O	1:B:66:ASN:HB3	1.97	0.64
1:A:166:LYS:HB3	1:A:176:TYR:CE2	2.32	0.64
1:B:140:GLY:HA3	1:B:170:ILE:CD1	2.28	0.64
1:A:244:VAL:O	1:A:244:VAL:HG23	1.96	0.64
1:A:58:GLU:C	1:A:59:ILE:HG23	2.16	0.64
1:B:163:LEU:CD2	1:B:167:LEU:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:O	1:A:201:GLN:HB2	1.98	0.64
1:B:122:GLN:HE22	1:B:124:GLY:HA3	1.58	0.64
1:B:127:ILE:CG2	1:B:128:ALA:N	2.21	0.64
1:B:174:GLU:HA	1:B:178:PRO:HA	1.80	0.64
1:A:253:SER:O	1:A:255:ALA:N	2.30	0.64
1:A:12:THR:HG23	1:A:269:ALA:CB	2.28	0.64
1:A:226:LYS:O	1:A:229:ILE:HG13	1.98	0.64
1:B:50:PRO:CB	1:B:128:ALA:HB3	2.23	0.64
1:B:143:ALA:HA	1:B:152:TRP:HA	1.78	0.64
1:B:83:PHE:O	1:B:278:TRP:CD1	2.51	0.64
1:A:277:LYS:CG	1:B:125:GLU:CD	2.67	0.64
1:B:112:VAL:C	1:B:150:THR:HB	2.11	0.64
1:B:173:VAL:HG13	1:B:177:PHE:HB2	1.79	0.64
1:A:47:VAL:CG2	1:A:131:GLY:H	2.11	0.64
1:A:42:ILE:CG2	1:A:159:ILE:CD1	2.76	0.64
1:A:174:GLU:HA	1:A:178:PRO:HA	1.80	0.64
1:B:12:THR:CG2	1:B:269:ALA:HB2	2.28	0.64
1:B:12:THR:HG23	1:B:269:ALA:CB	2.28	0.64
1:B:29:PHE:O	1:B:225:TRP:NE1	2.31	0.64
1:B:226:LYS:O	1:B:229:ILE:HG13	1.98	0.64
1:B:32:ILE:HG22	1:B:96:PRO:HG2	1.80	0.64
1:A:46:VAL:O	1:A:93:GLY:CA	2.44	0.63
1:B:252:TYR:CE1	1:B:254:LYS:HB2	2.33	0.63
1:A:177:PHE:HA	1:B:280:PHE:CE2	2.33	0.63
1:A:252:TYR:CE1	1:A:254:LYS:HB2	2.33	0.63
1:B:193:ILE:O	1:B:195:ASP:N	2.30	0.63
1:A:10:LYS:O	1:A:11:ASN:OD1	2.15	0.63
1:A:140:GLY:HA3	1:A:170:ILE:CD1	2.28	0.63
1:B:170:ILE:O	1:B:171:GLU:C	2.37	0.63
1:B:8:GLY:O	1:B:9:ALA:CB	2.46	0.63
1:A:25:PRO:HG2	1:A:257:SER:HA	1.81	0.63
1:A:8:GLY:O	1:A:9:ALA:CB	2.46	0.63
1:B:10:LYS:O	1:B:11:ASN:OD1	2.15	0.63
1:B:82:CYS:SG	1:B:190:ILE:CD1	2.87	0.63
1:B:200:ASN:O	1:B:201:GLN:HB2	1.98	0.63
1:A:139:LEU:O	1:A:211:LYS:HA	1.98	0.63
1:A:50:PRO:CB	1:A:128:ALA:HB3	2.23	0.63
1:A:163:LEU:HD22	1:A:177:PHE:HZ	1.60	0.63
1:A:190:ILE:CA	1:A:193:ILE:HD11	2.27	0.63
1:A:243:ASN:O	1:A:252:TYR:HA	1.97	0.63
1:A:83:PHE:O	1:A:278:TRP:CD1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:CE2	1:B:177:PHE:HA	2.33	0.63
1:B:58:GLU:C	1:B:59:ILE:CG2	2.66	0.63
1:B:11:ASN:HA	1:B:69:ILE:CD1	2.28	0.63
1:B:98:THR:HG21	1:B:221:THR:CG2	2.29	0.63
1:A:114:ASP:CB	1:A:149:GLU:OE1	2.45	0.63
1:B:9:ALA:HB1	1:B:15:TYR:CB	2.00	0.63
1:B:1:THR:CG2	1:B:26:VAL:HG21	2.27	0.63
1:B:25:PRO:HG2	1:B:257:SER:HA	1.81	0.63
1:A:220:GLU:HG2	1:A:220:GLU:O	1.96	0.63
1:B:158:ASP:C	1:B:160:ASN:N	2.49	0.63
1:B:163:LEU:HA	1:B:166:LYS:CD	2.28	0.63
1:B:54:ASN:H	1:B:54:ASN:HD22	1.46	0.63
1:B:9:ALA:HB2	1:B:15:TYR:CA	2.25	0.63
1:A:139:LEU:O	1:A:211:LYS:CA	2.45	0.63
1:B:139:LEU:CB	1:B:155:ILE:HG22	2.17	0.63
1:A:170:ILE:O	1:A:171:GLU:C	2.37	0.63
1:A:19:ILE:HD13	1:A:26:VAL:HG12	1.71	0.63
1:A:142:MET:N	1:A:153:LYS:O	2.31	0.63
1:A:26:VAL:CG2	1:A:27:SER:N	2.30	0.63
1:A:58:GLU:C	1:A:59:ILE:CG2	2.66	0.63
1:A:32:ILE:HG22	1:A:96:PRO:HG2	1.80	0.63
1:A:29:PHE:O	1:A:225:TRP:NE1	2.31	0.62
1:A:34:LEU:O	1:A:43:PHE:HB2	1.97	0.62
1:A:9:ALA:O	1:A:10:LYS:CB	2.36	0.62
1:A:125:GLU:CD	1:B:277:LYS:CG	2.66	0.62
1:A:158:ASP:C	1:A:160:ASN:N	2.49	0.62
1:A:25:PRO:CG	1:A:257:SER:HA	2.29	0.62
1:A:11:ASN:HA	1:A:69:ILE:CD1	2.29	0.62
1:B:163:LEU:HG	1:B:166:LYS:HD2	1.81	0.62
1:B:1:THR:O	1:B:2:TYR:HD1	1.81	0.62
1:B:249:THR:HG22	1:B:251:THR:OG1	1.99	0.62
1:A:9:ALA:HB1	1:A:15:TYR:CB	2.00	0.62
1:B:122:GLN:CG	1:B:157:ILE:HA	2.29	0.62
1:B:25:PRO:CG	1:B:257:SER:HA	2.29	0.62
1:A:222:HIS:NE2	1:A:226:LYS:CG	2.62	0.62
1:A:229:ILE:HG22	1:A:249:THR:HG21	1.81	0.62
1:A:12:THR:CG2	1:A:269:ALA:HB2	2.28	0.62
1:B:140:GLY:HA3	1:B:170:ILE:HD11	1.82	0.62
1:B:222:HIS:NE2	1:B:226:LYS:CG	2.62	0.62
1:A:163:LEU:HG	1:A:166:LYS:HD2	1.81	0.62
1:A:222:HIS:CD2	1:A:226:LYS:CG	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG21	1:A:221:THR:CG2	2.29	0.62
1:B:47:VAL:CG2	1:B:131:GLY:H	2.11	0.62
1:B:142:MET:HB2	1:B:153:LYS:HB2	1.78	0.62
1:A:1:THR:O	1:A:2:TYR:HD1	1.81	0.62
1:B:172:ASP:O	1:B:173:VAL:C	2.37	0.62
1:B:13:LEU:HG	1:B:76:LEU:HD21	1.82	0.62
1:B:86:HIS:CG	1:B:87:GLY:H	2.18	0.62
1:A:82:CYS:SG	1:A:190:ILE:CD1	2.87	0.62
1:B:42:ILE:CG2	1:B:159:ILE:CD1	2.76	0.62
1:B:229:ILE:HG22	1:B:249:THR:HG21	1.81	0.62
1:A:203:ALA:O	1:A:206:GLY:N	2.33	0.62
1:A:9:ALA:HB2	1:A:15:TYR:CA	2.25	0.62
1:A:99:TRP:O	1:A:224:SER:OG	2.18	0.62
1:A:90:HIS:CE1	1:A:184:THR:OG1	2.52	0.62
1:B:69:ILE:HG21	1:B:76:LEU:CB	2.26	0.62
1:A:106:HIS:HB2	1:A:107:PRO:HD2	1.82	0.62
1:A:105:SER:CB	1:A:109:THR:HG22	2.25	0.62
1:A:230:ALA:CB	1:A:233:SER:OG	2.48	0.62
1:B:158:ASP:CG	1:B:160:ASN:ND2	2.49	0.62
1:B:90:HIS:CE1	1:B:184:THR:OG1	2.53	0.62
1:A:13:LEU:HG	1:A:76:LEU:HD21	1.82	0.61
1:A:53:THR:O	1:A:88:TYR:CB	2.26	0.61
1:B:122:GLN:HE21	1:B:124:GLY:HA3	1.65	0.61
1:B:139:LEU:O	1:B:211:LYS:HA	1.98	0.61
1:A:48:GLU:O	1:A:49:ILE:CG1	2.43	0.61
1:B:275:ILE:O	1:B:276:ASP:C	2.38	0.61
1:A:122:GLN:CG	1:A:157:ILE:HA	2.29	0.61
1:A:141:ILE:CG2	1:A:141:ILE:O	2.43	0.61
1:A:172:ASP:O	1:A:173:VAL:C	2.37	0.61
1:A:97:GLN:HA	1:A:225:TRP:CE2	2.36	0.61
1:B:34:LEU:C	1:B:43:PHE:HB3	2.19	0.61
1:A:249:THR:HG22	1:A:251:THR:OG1	1.99	0.61
1:A:42:ILE:HG12	1:A:43:PHE:H	0.63	0.61
1:B:166:LYS:HB3	1:B:176:TYR:CZ	2.36	0.61
1:B:190:ILE:C	1:B:193:ILE:CG1	2.64	0.61
1:B:7:ILE:HB	1:B:16:LYS:C	2.19	0.61
1:B:203:ALA:O	1:B:206:GLY:N	2.33	0.61
1:A:209:LYS:HB3	1:A:213:TYR:HB2	1.82	0.61
1:A:275:ILE:O	1:A:276:ASP:C	2.38	0.61
1:B:97:GLN:HA	1:B:225:TRP:CE2	2.36	0.61
1:A:166:LYS:HB3	1:A:176:TYR:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:O	1:A:204:PHE:C	2.39	0.61
1:B:203:ALA:O	1:B:204:PHE:C	2.39	0.61
1:A:190:ILE:C	1:A:193:ILE:CG1	2.64	0.61
1:A:191:TYR:HE2	1:A:192:LYS:HE2	1.66	0.61
1:A:193:ILE:HA	1:A:197:LYS:O	2.01	0.61
1:A:7:ILE:HB	1:A:16:LYS:C	2.19	0.61
1:B:193:ILE:HA	1:B:197:LYS:O	2.01	0.61
1:A:86:HIS:CG	1:A:87:GLY:H	2.18	0.61
1:B:209:LYS:HB3	1:B:213:TYR:HB2	1.82	0.61
1:B:67:PRO:O	1:B:68:ILE:CG1	2.45	0.61
1:A:141:ILE:HD13	1:A:153:LYS:O	2.01	0.61
1:A:9:ALA:CB	1:A:15:TYR:N	2.63	0.61
1:B:142:MET:N	1:B:153:LYS:O	2.31	0.61
1:B:38:LYS:O	1:B:39:GLU:C	2.38	0.61
1:A:111:ALA:HB2	1:A:145:LEU:HD22	1.83	0.60
1:B:5:ARG:CZ	1:B:25:PRO:HB3	2.29	0.60
1:B:38:LYS:CD	1:B:41:ASN:HB2	2.31	0.60
1:B:99:TRP:O	1:B:224:SER:OG	2.18	0.60
1:A:101:ASP:O	1:A:113:GLY:HA3	2.02	0.60
1:A:4:THR:HG22	1:A:19:ILE:CB	2.31	0.60
1:A:6:GLN:OE1	1:A:265:PRO:HB2	2.01	0.60
1:A:38:LYS:O	1:A:39:GLU:C	2.38	0.60
1:B:34:LEU:O	1:B:43:PHE:HB2	1.97	0.60
1:A:139:LEU:CB	1:A:155:ILE:HG22	2.17	0.60
1:A:253:SER:C	1:A:255:ALA:N	2.55	0.60
1:A:122:GLN:HE21	1:A:124:GLY:CA	2.14	0.60
1:A:140:GLY:HA3	1:A:170:ILE:HD11	1.82	0.60
1:B:6:GLN:OE1	1:B:265:PRO:HB2	2.01	0.60
1:A:98:THR:HA	1:A:225:TRP:CB	2.31	0.60
1:A:56:LYS:NZ	1:A:70:GLN:NE2	2.50	0.60
1:A:92:TYR:CD2	1:A:121:LEU:HD23	2.37	0.60
1:B:122:GLN:HE21	1:B:124:GLY:CA	2.14	0.60
1:B:9:ALA:CB	1:B:15:TYR:N	2.63	0.60
1:B:106:HIS:HB2	1:B:107:PRO:HD2	1.82	0.60
1:A:104:VAL:O	1:A:105:SER:C	2.40	0.60
1:A:8:GLY:HA3	1:A:266:LYS:CG	2.29	0.60
1:A:125:GLU:CD	1:B:277:LYS:HG3	2.22	0.60
1:A:54:ASN:H	1:A:54:ASN:HD22	1.46	0.60
1:B:80:ARG:CG	1:B:194:PRO:HB2	2.25	0.60
1:B:4:THR:HG22	1:B:19:ILE:CB	2.31	0.60
1:A:158:ASP:CG	1:A:160:ASN:ND2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:O	1:A:183:ALA:CB	2.47	0.60
1:A:27:SER:O	1:A:31:ASP:N	2.35	0.60
1:B:179:GLY:O	1:B:183:ALA:CB	2.47	0.60
1:A:92:TYR:CD2	1:A:121:LEU:CD2	2.85	0.60
1:A:188:PHE:O	1:A:191:TYR:CB	2.48	0.60
1:A:19:ILE:HD12	1:A:26:VAL:CG1	2.16	0.60
1:B:141:ILE:HD13	1:B:153:LYS:O	2.01	0.60
1:B:9:ALA:O	1:B:10:LYS:CB	2.36	0.60
1:B:35:TYR:N	1:B:35:TYR:CD2	2.70	0.60
1:A:129:TYR:HD1	1:A:129:TYR:O	1.85	0.60
1:A:5:ARG:CZ	1:A:25:PRO:HB3	2.29	0.60
1:B:222:HIS:NE2	1:B:226:LYS:CD	2.62	0.60
1:A:157:ILE:HG23	1:A:158:ASP:N	2.17	0.59
1:A:222:HIS:CD2	1:A:226:LYS:CE	2.66	0.59
1:B:222:HIS:CD2	1:B:226:LYS:CG	2.82	0.59
1:B:56:LYS:NZ	1:B:70:GLN:NE2	2.50	0.59
1:B:29:PHE:H	1:B:96:PRO:CB	2.15	0.59
1:A:69:ILE:HG21	1:A:76:LEU:CB	2.26	0.59
1:B:92:TYR:CD2	1:B:121:LEU:HD23	2.36	0.59
1:B:27:SER:O	1:B:31:ASP:N	2.35	0.59
1:B:92:TYR:CD2	1:B:121:LEU:CD2	2.85	0.59
1:A:163:LEU:HB3	1:A:167:LEU:HD13	1.85	0.59
1:A:241:LEU:N	1:A:241:LEU:HD12	2.17	0.59
1:A:38:LYS:C	1:A:40:ASP:N	2.53	0.59
1:A:34:LEU:C	1:A:43:PHE:HB3	2.19	0.59
1:A:83:PHE:CB	1:A:84:PRO:CD	2.80	0.59
1:B:101:ASP:O	1:B:113:GLY:HA3	2.02	0.59
1:B:271:ILE:HB	1:B:275:ILE:HD12	1.84	0.59
1:B:38:LYS:C	1:B:40:ASP:N	2.53	0.59
1:B:253:SER:C	1:B:255:ALA:N	2.55	0.59
1:A:158:ASP:C	1:A:160:ASN:H	2.06	0.59
1:A:160:ASN:HD22	1:A:161:ASP:N	2.01	0.59
1:A:166:LYS:CD	1:A:176:TYR:CE2	2.81	0.59
1:A:29:PHE:H	1:A:96:PRO:CB	2.15	0.59
1:B:111:ALA:HB2	1:B:145:LEU:HD22	1.83	0.59
1:B:127:ILE:HG23	1:B:128:ALA:H	1.61	0.59
1:B:181:LEU:O	1:B:184:THR:N	2.28	0.59
1:B:19:ILE:HD12	1:B:26:VAL:CG1	2.16	0.59
1:B:59:ILE:O	1:B:59:ILE:HG13	2.02	0.59
1:B:49:ILE:CD1	1:B:92:TYR:HB3	2.32	0.59
1:A:38:LYS:CD	1:A:41:ASN:HB2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:C	1:B:160:ASN:H	2.06	0.59
1:B:42:ILE:HG12	1:B:43:PHE:CA	2.23	0.59
1:B:160:ASN:HD22	1:B:161:ASP:N	2.01	0.59
1:A:59:ILE:HG13	1:A:59:ILE:O	2.02	0.59
1:A:59:ILE:CG2	1:A:66:ASN:C	2.66	0.59
1:B:192:LYS:C	1:B:197:LYS:O	2.40	0.59
1:B:241:LEU:HD12	1:B:241:LEU:N	2.17	0.59
1:A:204:PHE:C	1:A:206:GLY:N	2.45	0.59
1:B:204:PHE:C	1:B:206:GLY:N	2.45	0.59
1:A:150:THR:CG2	1:A:150:THR:O	2.51	0.59
1:B:191:TYR:HE2	1:B:192:LYS:HE2	1.66	0.59
1:B:244:VAL:O	1:B:244:VAL:CG2	2.51	0.59
1:B:69:ILE:HD12	1:B:76:LEU:HG	1.85	0.59
1:B:83:PHE:CB	1:B:84:PRO:CD	2.80	0.59
1:A:192:LYS:CB	1:A:197:LYS:HB3	2.30	0.59
1:A:67:PRO:O	1:A:68:ILE:CG1	2.45	0.59
1:B:122:GLN:CG	1:B:156:ALA:O	2.51	0.59
1:B:157:ILE:HG23	1:B:158:ASP:N	2.17	0.59
1:B:141:ILE:HG13	1:B:217:ILE:HG21	1.85	0.59
1:B:65:LEU:C	1:B:66:ASN:CG	2.62	0.59
1:B:246:LEU:C	1:B:248:ASP:N	2.56	0.59
1:A:146:ASP:HB2	1:A:147:GLU:OE1	2.03	0.58
1:A:7:ILE:CG2	1:A:14:GLU:O	2.51	0.58
1:A:277:LYS:HG3	1:B:125:GLU:CD	2.22	0.58
1:B:129:TYR:O	1:B:129:TYR:HD1	1.85	0.58
1:B:41:ASN:HD21	1:B:137:LYS:CE	2.10	0.58
1:B:58:GLU:O	1:B:59:ILE:CG2	2.52	0.58
1:A:51:ARG:CG	1:A:90:HIS:N	2.64	0.58
1:B:7:ILE:CG2	1:B:14:GLU:O	2.51	0.58
1:B:19:ILE:HD13	1:B:19:ILE:C	2.24	0.58
1:A:192:LYS:C	1:A:197:LYS:O	2.40	0.58
1:A:122:GLN:CG	1:A:156:ALA:O	2.51	0.58
1:A:69:ILE:HD12	1:A:76:LEU:HG	1.85	0.58
1:B:150:THR:CG2	1:B:150:THR:O	2.51	0.58
1:A:141:ILE:HG13	1:A:217:ILE:HG21	1.85	0.58
1:A:244:VAL:CG2	1:A:244:VAL:O	2.51	0.58
1:B:104:VAL:O	1:B:105:SER:C	2.40	0.58
1:B:163:LEU:HB3	1:B:167:LEU:HD13	1.85	0.58
1:B:98:THR:HA	1:B:225:TRP:CB	2.31	0.58
1:A:217:ILE:HG23	1:A:218:ILE:N	2.18	0.58
1:A:110:LYS:C	1:A:112:VAL:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:OE2	1:A:256:ALA:HB1	2.04	0.58
1:A:49:ILE:CD1	1:A:92:TYR:HB3	2.32	0.58
1:B:122:GLN:HG2	1:B:157:ILE:HA	1.86	0.58
1:B:164:ALA:C	1:B:166:LYS:H	2.07	0.58
1:B:80:ARG:NE	1:B:80:ARG:HA	2.19	0.58
1:B:98:THR:OG1	1:B:221:THR:HG23	2.04	0.58
1:A:127:ILE:HG23	1:A:128:ALA:H	1.61	0.58
1:A:80:ARG:HD3	1:A:279:PHE:CD1	2.37	0.58
1:A:34:LEU:C	1:A:36:ALA:H	2.06	0.58
1:A:41:ASN:HD21	1:A:137:LYS:CE	2.10	0.58
1:A:18:TYR:CE1	1:A:260:ILE:HD12	2.39	0.58
1:A:65:LEU:C	1:A:66:ASN:CG	2.62	0.58
1:B:103:ASN:HA	1:B:112:VAL:CG1	2.33	0.58
1:B:99:TRP:CZ2	1:B:115:ASN:OD1	2.57	0.58
1:B:97:GLN:C	1:B:225:TRP:CG	2.78	0.58
1:B:48:GLU:O	1:B:49:ILE:CG1	2.43	0.58
1:A:74:GLY:O	1:A:75:LYS:HG2	1.96	0.58
1:B:71:ASN:C	1:B:72:THR:OG1	2.43	0.58
1:A:193:ILE:CA	1:A:197:LYS:O	2.52	0.57
1:A:19:ILE:HD13	1:A:19:ILE:C	2.24	0.57
1:B:63:GLU:OE2	1:B:256:ALA:HB1	2.04	0.57
1:A:99:TRP:CZ2	1:A:115:ASN:OD1	2.57	0.57
1:A:157:ILE:HG23	1:A:158:ASP:H	1.69	0.57
1:A:141:ILE:HG13	1:A:214:ALA:HA	1.86	0.57
1:A:246:LEU:C	1:A:248:ASP:N	2.56	0.57
1:B:110:LYS:C	1:B:112:VAL:N	2.37	0.57
1:A:142:MET:HB2	1:A:153:LYS:HB2	1.78	0.57
1:A:225:TRP:CE3	1:A:226:LYS:N	2.73	0.57
1:A:225:TRP:CH2	1:A:229:ILE:HD11	2.39	0.57
1:A:271:ILE:HB	1:A:275:ILE:HD12	1.84	0.57
1:B:225:TRP:CH2	1:B:229:ILE:HD11	2.39	0.57
1:B:80:ARG:HD3	1:B:279:PHE:CD1	2.37	0.57
1:A:54:ASN:HB2	1:A:275:ILE:HG21	1.86	0.57
1:B:90:HIS:CE1	1:B:184:THR:HG23	2.40	0.57
1:B:54:ASN:OD1	1:B:81:ASN:CG	2.43	0.57
1:A:122:GLN:HE21	1:A:124:GLY:HA3	1.65	0.57
1:A:187:TRP:O	1:A:187:TRP:CE3	2.57	0.57
1:A:98:THR:OG1	1:A:221:THR:HG23	2.04	0.57
1:A:228:LEU:CD1	1:A:234:SER:OG	2.53	0.57
1:A:86:HIS:CG	1:A:87:GLY:N	2.71	0.57
1:A:97:GLN:C	1:A:225:TRP:CG	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:HB3	1:A:15:TYR:CD1	2.39	0.57
1:A:107:PRO:O	1:A:108:GLU:CB	2.52	0.57
1:B:107:PRO:O	1:B:108:GLU:CB	2.52	0.57
1:A:158:ASP:OD2	1:A:160:ASN:ND2	2.38	0.57
1:A:58:GLU:O	1:A:59:ILE:CG2	2.52	0.57
1:B:9:ALA:HB3	1:B:15:TYR:CD1	2.39	0.57
1:B:146:ASP:HB2	1:B:147:GLU:OE1	2.03	0.57
1:A:57:LEU:HB3	1:A:68:ILE:H	1.69	0.57
1:B:228:LEU:CD1	1:B:234:SER:OG	2.53	0.57
1:B:158:ASP:CB	1:B:161:ASP:HB3	2.35	0.57
1:B:187:TRP:O	1:B:187:TRP:CE3	2.57	0.57
1:B:193:ILE:CA	1:B:197:LYS:O	2.52	0.57
1:B:230:ALA:CB	1:B:233:SER:OG	2.48	0.57
1:B:18:TYR:CE1	1:B:260:ILE:HD12	2.39	0.57
1:B:86:HIS:CG	1:B:87:GLY:N	2.71	0.57
1:A:222:HIS:NE2	1:A:226:LYS:CD	2.62	0.56
1:B:58:GLU:CD	1:B:116:ASN:OD1	2.43	0.56
1:B:158:ASP:OD2	1:B:160:ASN:ND2	2.38	0.56
1:B:19:ILE:HD13	1:B:26:VAL:HG12	1.71	0.56
1:B:225:TRP:CE3	1:B:226:LYS:N	2.73	0.56
1:B:5:ARG:HH12	1:B:260:ILE:HG21	0.72	0.56
1:B:8:GLY:H	1:B:265:PRO:HA	1.69	0.56
1:A:242:THR:CA	1:A:251:THR:HB	2.32	0.56
1:B:98:THR:HG22	1:B:221:THR:OG1	1.93	0.56
1:B:137:LYS:HE3	1:B:159:ILE:HG23	1.88	0.56
1:B:141:ILE:HG13	1:B:214:ALA:HA	1.86	0.56
1:B:54:ASN:HB2	1:B:275:ILE:HG21	1.86	0.56
1:A:137:LYS:HE3	1:A:159:ILE:HG23	1.88	0.56
1:A:112:VAL:C	1:A:150:THR:HB	2.11	0.56
1:A:229:ILE:O	1:A:231:GLY:N	2.38	0.56
1:A:54:ASN:OD1	1:A:81:ASN:CG	2.43	0.56
1:B:157:ILE:HG23	1:B:158:ASP:H	1.69	0.56
1:A:122:GLN:HG2	1:A:157:ILE:HA	1.86	0.56
1:A:164:ALA:C	1:A:166:LYS:H	2.07	0.56
1:A:90:HIS:CE1	1:A:184:THR:HG23	2.40	0.56
1:B:33:PRO:HA	1:B:97:GLN:NE2	2.20	0.56
1:A:218:ILE:HG22	1:A:219:LYS:N	2.19	0.56
1:B:229:ILE:O	1:B:231:GLY:N	2.38	0.56
1:B:64:THR:C	1:B:65:LEU:CD2	2.72	0.56
1:A:42:ILE:HG12	1:A:43:PHE:CA	2.23	0.56
1:A:58:GLU:CD	1:A:116:ASN:OD1	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:CB	1:A:15:TYR:HA	2.31	0.56
1:A:90:HIS:O	1:A:91:ASN:CB	2.41	0.56
1:B:82:CYS:HG	1:B:190:ILE:HG13	1.66	0.56
1:B:217:ILE:HG23	1:B:218:ILE:N	2.18	0.56
1:A:8:GLY:H	1:A:265:PRO:HA	1.70	0.56
1:A:80:ARG:NE	1:A:80:ARG:HA	2.19	0.56
1:A:12:THR:OG1	1:A:13:LEU:N	2.39	0.56
1:B:158:ASP:O	1:B:159:ILE:C	2.44	0.56
1:B:218:ILE:HG22	1:B:219:LYS:N	2.19	0.56
1:B:45:MET:HE2	1:B:120:VAL:CG1	2.21	0.56
1:A:139:LEU:HD12	1:A:155:ILE:HG21	1.89	0.56
1:B:192:LYS:CB	1:B:197:LYS:HB3	2.30	0.55
1:B:20:GLU:HA	1:B:26:VAL:HG12	1.88	0.55
1:B:59:ILE:CG2	1:B:66:ASN:C	2.66	0.55
1:A:103:ASN:O	1:A:104:VAL:CB	2.28	0.55
1:A:32:ILE:O	1:A:32:ILE:HG22	2.06	0.55
1:A:33:PRO:HA	1:A:97:GLN:NE2	2.20	0.55
1:B:105:SER:CB	1:B:109:THR:HG22	2.25	0.55
1:A:35:TYR:N	1:A:35:TYR:CD2	2.70	0.55
1:A:103:ASN:HA	1:A:112:VAL:CG1	2.33	0.55
1:A:4:THR:CA	1:A:19:ILE:HA	2.37	0.55
1:B:12:THR:OG1	1:B:13:LEU:N	2.39	0.55
1:B:225:TRP:HE3	1:B:226:LYS:N	2.04	0.55
1:B:107:PRO:O	1:B:108:GLU:HB2	2.07	0.55
1:B:34:LEU:C	1:B:36:ALA:H	2.06	0.55
1:B:59:ILE:HG22	1:B:67:PRO:CD	2.34	0.55
1:A:158:ASP:CB	1:A:161:ASP:HB3	2.35	0.55
1:A:232:LYS:O	1:A:234:SER:O	2.25	0.55
1:A:30:HIS:HB3	1:A:243:ASN:OD1	2.06	0.55
1:A:25:PRO:HG3	1:A:257:SER:CA	2.37	0.55
1:A:241:LEU:O	1:A:243:ASN:CG	2.44	0.55
1:B:4:THR:CA	1:B:19:ILE:HA	2.37	0.55
1:A:211:LYS:HD3	1:A:212:LYS:NZ	2.22	0.55
1:A:225:TRP:HE3	1:A:226:LYS:N	2.04	0.55
1:A:7:ILE:HG22	1:A:15:TYR:CA	2.35	0.55
1:B:181:LEU:O	1:B:183:ALA:N	2.40	0.55
1:B:30:HIS:HB3	1:B:243:ASN:OD1	2.06	0.55
1:B:6:GLN:HB3	1:B:265:PRO:HB3	1.88	0.55
1:B:8:GLY:HA3	1:B:266:LYS:CG	2.29	0.55
1:A:61:LYS:HG3	1:A:239:ILE:HG22	1.88	0.55
1:A:95:PHE:CE2	1:A:154:VAL:HG11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:O	1:B:234:SER:O	2.25	0.55
1:B:57:LEU:HB3	1:B:68:ILE:H	1.69	0.55
1:A:139:LEU:CD1	1:A:155:ILE:HG21	2.37	0.55
1:B:139:LEU:HD12	1:B:155:ILE:HG21	1.89	0.55
1:A:158:ASP:O	1:A:159:ILE:C	2.44	0.55
1:A:6:GLN:HB3	1:A:265:PRO:HB3	1.88	0.55
1:B:166:LYS:CD	1:B:176:TYR:CE2	2.81	0.55
1:B:95:PHE:CE2	1:B:154:VAL:HG11	2.42	0.55
1:A:107:PRO:O	1:A:108:GLU:HB2	2.07	0.55
1:A:226:LYS:C	1:A:228:LEU:H	2.11	0.54
1:A:25:PRO:HG3	1:A:257:SER:O	2.07	0.54
1:A:58:GLU:N	1:A:68:ILE:H	2.05	0.54
1:B:11:ASN:O	1:B:13:LEU:N	2.40	0.54
1:B:25:PRO:HG3	1:B:257:SER:CA	2.37	0.54
1:B:58:GLU:N	1:B:68:ILE:H	2.05	0.54
1:A:139:LEU:CG	1:A:155:ILE:CG2	2.86	0.54
1:B:241:LEU:O	1:B:243:ASN:CG	2.44	0.54
1:B:211:LYS:HD3	1:B:212:LYS:NZ	2.22	0.54
1:A:71:ASN:C	1:A:72:THR:OG1	2.43	0.54
1:B:147:GLU:O	1:B:148:GLY:C	2.45	0.54
1:A:142:MET:HE2	1:A:202:PHE:HE1	1.64	0.54
1:B:9:ALA:CB	1:B:15:TYR:HA	2.31	0.54
1:B:173:VAL:HA	1:B:177:PHE:HD1	1.73	0.54
1:B:139:LEU:CD1	1:B:155:ILE:HG21	2.37	0.54
1:A:181:LEU:O	1:A:183:ALA:N	2.40	0.54
1:A:11:ASN:O	1:A:13:LEU:N	2.40	0.54
1:B:11:ASN:HA	1:B:69:ILE:HD11	1.89	0.54
1:B:184:THR:O	1:B:185:ASP:C	2.46	0.54
1:B:153:LYS:HE2	1:B:188:PHE:CZ	2.43	0.54
1:B:40:ASP:OD2	1:B:40:ASP:N	2.41	0.54
1:B:61:LYS:HG3	1:B:239:ILE:HG22	1.88	0.54
1:A:147:GLU:O	1:A:148:GLY:C	2.45	0.54
1:A:153:LYS:HE2	1:A:188:PHE:CZ	2.43	0.54
1:B:54:ASN:N	1:B:54:ASN:ND2	2.56	0.54
1:A:228:LEU:HD12	1:A:234:SER:OG	2.08	0.54
1:B:173:VAL:O	1:B:176:TYR:N	2.41	0.54
1:A:92:TYR:HA	1:A:120:VAL:O	2.08	0.54
1:A:129:TYR:O	1:A:131:GLY:N	2.41	0.54
1:B:92:TYR:HA	1:B:120:VAL:O	2.08	0.54
1:B:92:TYR:HE2	1:B:121:LEU:HD21	1.73	0.54
1:B:139:LEU:CG	1:B:155:ILE:CG2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:CB	1:A:16:LYS:H	2.15	0.54
1:A:173:VAL:O	1:A:176:TYR:N	2.41	0.54
1:A:173:VAL:HA	1:A:177:PHE:HD1	1.73	0.54
1:A:98:THR:C	1:A:225:TRP:HB2	2.29	0.54
1:A:64:THR:C	1:A:65:LEU:CD2	2.72	0.54
1:A:11:ASN:HA	1:A:69:ILE:HD11	1.89	0.54
1:A:139:LEU:CD1	1:A:155:ILE:CG2	2.85	0.54
1:A:176:TYR:HB3	1:A:177:PHE:CD1	2.43	0.53
1:A:20:GLU:HA	1:A:26:VAL:HG12	1.88	0.53
1:B:176:TYR:HB3	1:B:177:PHE:CD1	2.43	0.53
1:A:229:ILE:HG22	1:A:249:THR:CG2	2.38	0.53
1:A:244:VAL:HG21	1:A:254:LYS:HG3	1.90	0.53
1:A:98:THR:HG22	1:A:221:THR:OG1	1.93	0.53
1:A:5:ARG:HH12	1:A:260:ILE:HG21	0.72	0.53
1:B:25:PRO:HG3	1:B:257:SER:O	2.07	0.53
1:B:49:ILE:CG1	1:B:92:TYR:CB	2.86	0.53
1:A:1:THR:CB	1:A:133:VAL:HG21	2.38	0.53
1:B:228:LEU:HD12	1:B:234:SER:OG	2.08	0.53
1:B:89:ILE:O	1:B:90:HIS:CG	2.61	0.53
1:A:122:GLN:HB2	1:A:156:ALA:O	2.07	0.53
1:A:184:THR:HA	1:A:187:TRP:HD1	1.74	0.53
1:A:54:ASN:ND2	1:A:54:ASN:N	2.56	0.53
1:B:188:PHE:O	1:B:191:TYR:CB	2.48	0.53
1:B:229:ILE:HG22	1:B:249:THR:CG2	2.38	0.53
1:B:254:LYS:HG2	1:B:254:LYS:O	2.08	0.53
1:B:32:ILE:O	1:B:32:ILE:HG22	2.06	0.53
1:A:182:ARG:HH11	1:A:185:ASP:HB2	1.72	0.53
1:B:129:TYR:O	1:B:131:GLY:N	2.41	0.53
1:B:1:THR:CB	1:B:133:VAL:HG21	2.38	0.53
1:B:222:HIS:CD2	1:B:226:LYS:CE	2.66	0.53
1:A:9:ALA:HB2	1:A:15:TYR:N	2.24	0.53
1:A:184:THR:O	1:A:185:ASP:C	2.46	0.53
1:A:40:ASP:N	1:A:40:ASP:OD2	2.41	0.53
1:B:184:THR:HA	1:B:187:TRP:HD1	1.74	0.53
1:B:32:ILE:O	1:B:33:PRO:O	2.27	0.53
1:B:29:PHE:N	1:B:96:PRO:HB2	2.24	0.53
1:A:159:ILE:O	1:A:159:ILE:HG22	2.09	0.53
1:A:89:ILE:O	1:A:90:HIS:CG	2.61	0.53
1:B:226:LYS:C	1:B:228:LEU:H	2.11	0.53
1:B:90:HIS:CE1	1:B:184:THR:HG1	2.26	0.53
1:B:81:ASN:ND2	1:B:276:ASP:HA	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASN:OD1	1:B:81:ASN:OD1	2.27	0.53
1:A:254:LYS:O	1:A:254:LYS:HG2	2.09	0.52
1:A:81:ASN:ND2	1:A:276:ASP:HA	2.24	0.52
1:A:181:LEU:O	1:A:184:THR:N	2.28	0.52
1:A:142:MET:HG3	1:A:208:ALA:HB2	1.91	0.52
1:A:49:ILE:CG1	1:A:92:TYR:CB	2.86	0.52
1:B:7:ILE:HG22	1:B:15:TYR:CA	2.35	0.52
1:A:2:TYR:CB	1:A:22:ASP:H	2.22	0.52
1:A:54:ASN:OD1	1:A:81:ASN:OD1	2.27	0.52
1:A:59:ILE:HG22	1:A:67:PRO:CD	2.34	0.52
1:B:29:PHE:HE1	1:B:225:TRP:HD1	1.53	0.52
1:B:32:ILE:CG2	1:B:96:PRO:CG	2.79	0.52
1:B:48:GLU:HB3	1:B:67:PRO:HB3	1.91	0.52
1:B:51:ARG:CB	1:B:51:ARG:CZ	2.87	0.52
1:A:32:ILE:O	1:A:33:PRO:O	2.27	0.52
1:B:118:ILE:HG23	1:B:119:ASP:N	2.23	0.52
1:B:122:GLN:HG3	1:B:157:ILE:HA	1.91	0.52
1:B:7:ILE:CB	1:B:16:LYS:H	2.15	0.52
1:A:27:SER:OG	1:A:30:HIS:HB2	2.10	0.52
1:B:50:PRO:HA	1:B:128:ALA:CB	2.39	0.52
1:B:98:THR:C	1:B:225:TRP:HB2	2.29	0.52
1:B:106:HIS:CG	1:B:107:PRO:HD2	2.45	0.52
1:A:122:GLN:HG3	1:A:157:ILE:HA	1.91	0.52
1:B:159:ILE:HG22	1:B:159:ILE:O	2.09	0.52
1:B:209:LYS:CB	1:B:213:TYR:HB2	2.39	0.52
1:B:27:SER:OG	1:B:30:HIS:HB2	2.10	0.52
1:B:244:VAL:HG21	1:B:254:LYS:HG3	1.90	0.52
1:B:64:THR:O	1:B:64:THR:HG22	2.09	0.52
1:A:238:GLY:O	1:A:239:ILE:HD13	2.10	0.52
1:B:122:GLN:HB2	1:B:156:ALA:O	2.07	0.52
1:B:190:ILE:O	1:B:193:ILE:HG12	2.10	0.52
1:B:21:LYS:HB3	1:B:26:VAL:HB	1.92	0.52
1:A:116:ASN:O	1:A:117:PRO:O	2.28	0.52
1:A:171:GLU:O	1:A:172:ASP:C	2.48	0.52
1:A:21:LYS:HB3	1:A:26:VAL:HB	1.92	0.52
1:A:48:GLU:HB3	1:A:67:PRO:HB3	1.91	0.52
1:B:142:MET:HG3	1:B:208:ALA:HB2	1.91	0.52
1:B:249:THR:C	1:B:251:THR:N	2.59	0.52
1:B:69:ILE:HG22	1:B:77:ARG:N	2.20	0.52
1:B:139:LEU:CD1	1:B:155:ILE:CG2	2.85	0.52
1:A:16:LYS:CE	1:A:62:GLU:OE2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:CG2	1:A:67:PRO:CA	2.83	0.51
1:A:92:TYR:HE2	1:A:121:LEU:HD21	1.73	0.51
1:A:54:ASN:N	1:A:54:ASN:HD22	2.08	0.51
1:B:54:ASN:N	1:B:54:ASN:HD22	2.08	0.51
1:B:51:ARG:HA	1:B:88:TYR:O	2.10	0.51
1:B:2:TYR:CB	1:B:22:ASP:H	2.22	0.51
1:B:16:LYS:CE	1:B:62:GLU:OE2	2.58	0.51
1:B:74:GLY:O	1:B:75:LYS:HG2	1.96	0.51
1:A:105:SER:CB	1:A:109:THR:O	2.57	0.51
1:A:209:LYS:CB	1:A:213:TYR:HB2	2.39	0.51
1:A:29:PHE:N	1:A:96:PRO:HB2	2.24	0.51
1:B:161:ASP:CG	1:B:162:PRO:HD2	2.31	0.51
1:B:238:GLY:O	1:B:239:ILE:HD13	2.10	0.51
1:A:50:PRO:HA	1:A:128:ALA:CB	2.39	0.51
1:A:51:ARG:HA	1:A:88:TYR:O	2.10	0.51
1:B:171:GLU:O	1:B:172:ASP:C	2.48	0.51
1:B:46:VAL:HG13	1:B:96:PRO:HG3	1.92	0.51
1:B:51:ARG:CG	1:B:90:HIS:N	2.64	0.51
1:B:58:GLU:O	1:B:66:ASN:O	2.29	0.51
1:A:65:LEU:C	1:A:66:ASN:ND2	2.63	0.51
1:B:9:ALA:HB2	1:B:15:TYR:N	2.24	0.51
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.45	0.51
1:A:51:ARG:CZ	1:A:51:ARG:HB2	2.40	0.51
1:B:192:LYS:HE3	1:B:200:ASN:OD1	2.11	0.51
1:B:242:THR:CA	1:B:251:THR:HB	2.32	0.51
1:B:38:LYS:HG2	1:B:41:ASN:N	2.26	0.51
1:B:51:ARG:HB2	1:B:51:ARG:CZ	2.40	0.51
1:A:89:ILE:O	1:A:90:HIS:ND1	2.44	0.51
1:B:111:ALA:HB1	1:B:149:GLU:N	2.26	0.51
1:A:46:VAL:HG13	1:A:96:PRO:HG3	1.93	0.51
1:A:64:THR:O	1:A:64:THR:CG2	2.59	0.51
1:B:105:SER:CB	1:B:109:THR:O	2.57	0.51
1:B:115:ASN:C	1:B:116:ASN:O	2.49	0.51
1:B:5:ARG:HH11	1:B:260:ILE:CG2	1.87	0.51
1:A:192:LYS:O	1:A:193:ILE:C	2.49	0.51
1:A:47:VAL:O	1:A:131:GLY:N	2.44	0.51
1:A:90:HIS:CE1	1:A:184:THR:HG1	2.27	0.51
1:A:1:THR:H3	1:A:133:VAL:CG1	2.23	0.50
1:A:64:THR:HG22	1:A:64:THR:O	2.09	0.50
1:A:86:HIS:ND1	1:A:87:GLY:N	2.59	0.50
1:B:173:VAL:O	1:B:174:GLU:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:O	1:B:193:ILE:C	2.50	0.50
1:B:47:VAL:O	1:B:131:GLY:N	2.43	0.50
1:A:129:TYR:CD2	1:A:132:GLN:CD	2.85	0.50
1:A:38:LYS:HG2	1:A:41:ASN:N	2.26	0.50
1:B:142:MET:HE1	1:B:202:PHE:CZ	2.34	0.50
1:B:38:LYS:HG2	1:B:38:LYS:O	2.11	0.50
1:A:190:ILE:O	1:A:193:ILE:HG12	2.10	0.50
1:A:38:LYS:HG2	1:A:38:LYS:O	2.11	0.50
1:B:89:ILE:O	1:B:90:HIS:ND1	2.44	0.50
1:A:161:ASP:CG	1:A:162:PRO:HD2	2.31	0.50
1:A:173:VAL:O	1:A:174:GLU:C	2.49	0.50
1:B:116:ASN:O	1:B:117:PRO:O	2.28	0.50
1:B:11:ASN:HA	1:B:69:ILE:HD12	1.94	0.50
1:A:62:GLU:O	1:A:63:GLU:CB	2.44	0.50
1:B:129:TYR:CD2	1:B:132:GLN:CD	2.85	0.50
1:B:69:ILE:C	1:B:70:GLN:O	2.45	0.50
1:A:192:LYS:HE3	1:A:200:ASN:OD1	2.11	0.50
1:A:252:TYR:HE1	1:A:254:LYS:HB2	1.76	0.50
1:B:241:LEU:O	1:B:242:THR:O	2.30	0.50
1:B:8:GLY:CA	1:B:266:LYS:N	2.73	0.50
1:A:115:ASN:C	1:A:116:ASN:O	2.49	0.50
1:A:58:GLU:O	1:A:66:ASN:O	2.29	0.50
1:A:8:GLY:CA	1:A:266:LYS:N	2.73	0.50
1:A:65:LEU:O	1:A:66:ASN:CG	2.50	0.49
1:B:164:ALA:C	1:B:166:LYS:N	2.65	0.49
1:B:197:LYS:O	1:B:198:PRO:O	2.30	0.49
1:B:42:ILE:HG13	1:B:136:VAL:C	2.10	0.49
1:B:51:ARG:CA	1:B:88:TYR:O	2.59	0.49
1:A:142:MET:HB2	1:A:153:LYS:CB	2.38	0.49
1:A:142:MET:HE2	1:A:202:PHE:HZ	1.56	0.49
1:A:3:THR:O	1:A:20:GLU:CA	2.60	0.49
1:B:142:MET:CE	1:B:202:PHE:HE1	2.16	0.49
1:B:142:MET:HE2	1:B:202:PHE:HE1	1.73	0.49
1:B:86:HIS:ND1	1:B:87:GLY:N	2.59	0.49
1:A:111:ALA:HB1	1:A:149:GLU:N	2.26	0.49
1:A:127:ILE:CG2	1:A:128:ALA:N	2.21	0.49
1:A:4:THR:HG22	1:A:19:ILE:HA	1.93	0.49
1:A:97:GLN:O	1:A:225:TRP:CE3	2.65	0.49
1:A:51:ARG:CA	1:A:88:TYR:O	2.59	0.49
1:B:141:ILE:O	1:B:208:ALA:HB1	2.12	0.49
1:B:147:GLU:O	1:B:149:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:CG1	1:B:254:LYS:HA	2.42	0.49
1:B:64:THR:O	1:B:64:THR:CG2	2.59	0.49
1:A:125:GLU:CD	1:B:277:LYS:HG2	2.33	0.49
1:A:241:LEU:O	1:A:242:THR:O	2.30	0.49
1:B:43:PHE:CZ	1:B:218:ILE:HD13	2.47	0.49
1:B:34:LEU:HG	1:B:96:PRO:O	2.12	0.49
1:A:213:TYR:O	1:A:217:ILE:HB	2.13	0.49
1:B:47:VAL:C	1:B:48:GLU:HG3	2.32	0.49
1:A:69:ILE:C	1:A:70:GLN:O	2.45	0.49
1:A:94:ALA:O	1:A:95:PHE:C	2.51	0.49
1:A:34:LEU:HG	1:A:96:PRO:O	2.12	0.49
1:B:226:LYS:C	1:B:228:LEU:N	2.65	0.49
1:A:111:ALA:HB3	1:A:145:LEU:CD2	2.43	0.49
1:B:97:GLN:O	1:B:225:TRP:CE3	2.65	0.49
1:A:147:GLU:O	1:A:149:GLU:HG2	2.12	0.49
1:A:164:ALA:C	1:A:166:LYS:N	2.65	0.49
1:A:70:GLN:O	1:A:77:ARG:HB2	2.13	0.49
1:B:111:ALA:HB3	1:B:145:LEU:CD2	2.43	0.49
1:B:177:PHE:HD1	1:B:177:PHE:N	2.08	0.49
1:B:217:ILE:HG22	1:B:218:ILE:N	2.27	0.49
1:B:5:ARG:HH22	1:B:25:PRO:CB	2.20	0.49
1:B:59:ILE:CG2	1:B:67:PRO:CA	2.83	0.49
1:A:109:THR:CG2	1:A:150:THR:OG1	2.49	0.49
1:A:181:LEU:C	1:A:183:ALA:N	2.66	0.49
1:B:213:TYR:O	1:B:217:ILE:HB	2.13	0.49
1:A:118:ILE:HG23	1:A:119:ASP:N	2.23	0.49
1:B:182:ARG:HH11	1:B:185:ASP:HB2	1.72	0.49
1:B:3:THR:O	1:B:20:GLU:CA	2.60	0.49
1:B:27:SER:HB3	1:B:31:ASP:OD2	2.13	0.49
1:B:49:ILE:HG13	1:B:92:TYR:CB	2.35	0.49
1:A:158:ASP:HB3	1:A:160:ASN:HD22	1.78	0.48
1:A:177:PHE:N	1:A:177:PHE:HD1	2.07	0.48
1:A:43:PHE:CZ	1:A:218:ILE:HD13	2.47	0.48
1:A:188:PHE:O	1:A:191:TYR:CD2	2.67	0.48
1:A:83:PHE:CD2	1:A:84:PRO:N	2.81	0.48
1:B:99:TRP:HZ2	1:B:115:ASN:OD1	1.96	0.48
1:B:142:MET:HB2	1:B:153:LYS:CB	2.38	0.48
1:B:190:ILE:N	1:B:193:ILE:HD11	2.28	0.48
1:B:63:GLU:O	1:B:240:ASP:HB3	2.13	0.48
1:A:137:LYS:HG3	1:A:159:ILE:CD1	2.44	0.48
1:A:226:LYS:C	1:A:228:LEU:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:C	1:A:48:GLU:HG3	2.32	0.48
1:B:160:ASN:H	1:B:160:ASN:ND2	2.10	0.48
1:B:225:TRP:C	1:B:225:TRP:CE3	2.87	0.48
1:A:141:ILE:O	1:A:208:ALA:HB1	2.12	0.48
1:A:225:TRP:CE3	1:A:225:TRP:C	2.87	0.48
1:B:177:PHE:N	1:B:178:PRO:CD	2.76	0.48
1:B:190:ILE:O	1:B:193:ILE:CG1	2.61	0.48
1:A:177:PHE:N	1:A:178:PRO:CD	2.76	0.48
1:A:190:ILE:N	1:A:193:ILE:HD11	2.29	0.48
1:A:1:THR:N	1:A:133:VAL:CG1	2.60	0.48
1:B:105:SER:HB2	1:B:112:VAL:CA	2.24	0.48
1:B:209:LYS:CB	1:B:213:TYR:CB	2.92	0.48
1:B:94:ALA:O	1:B:95:PHE:C	2.51	0.48
1:A:209:LYS:CB	1:A:213:TYR:CB	2.92	0.48
1:A:37:ASP:O	1:A:38:LYS:HB3	2.12	0.48
1:A:83:PHE:CA	1:A:278:TRP:CD1	2.94	0.48
1:B:70:GLN:O	1:B:77:ARG:HB2	2.13	0.48
1:A:5:ARG:HH11	1:A:260:ILE:CG2	1.87	0.48
1:B:158:ASP:HB3	1:B:160:ASN:HD22	1.78	0.48
1:B:41:ASN:C	1:B:42:ILE:HG22	2.33	0.48
1:B:83:PHE:CD2	1:B:84:PRO:N	2.81	0.48
1:B:84:PRO:O	1:B:85:HIS:HB2	2.12	0.48
1:A:11:ASN:HA	1:A:69:ILE:HD12	1.94	0.48
1:A:122:GLN:HG3	1:A:136:VAL:HG21	1.96	0.48
1:A:217:ILE:HG22	1:A:218:ILE:N	2.27	0.48
1:A:63:GLU:O	1:A:240:ASP:HB3	2.13	0.48
1:B:1:THR:HG22	1:B:26:VAL:HG11	1.91	0.48
1:A:4:THR:HG22	1:A:19:ILE:CA	2.44	0.48
1:A:244:VAL:CG1	1:A:254:LYS:HA	2.43	0.48
1:A:27:SER:HB3	1:A:31:ASP:OD2	2.13	0.48
1:A:69:ILE:HG22	1:A:77:ARG:N	2.20	0.48
1:B:4:THR:HG22	1:B:19:ILE:HA	1.93	0.48
1:B:37:ASP:O	1:B:38:LYS:HB3	2.12	0.48
1:A:190:ILE:O	1:A:193:ILE:CG1	2.61	0.48
1:A:41:ASN:C	1:A:42:ILE:HG22	2.33	0.48
1:B:129:TYR:O	1:B:129:TYR:CD1	2.67	0.48
1:B:111:ALA:CB	1:B:145:LEU:HD22	2.44	0.48
1:B:136:VAL:HA	1:B:159:ILE:H	1.79	0.48
1:B:163:LEU:HD22	1:B:177:PHE:CE1	2.48	0.48
1:A:136:VAL:HA	1:A:159:ILE:H	1.79	0.47
1:A:277:LYS:HG2	1:B:125:GLU:CD	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASN:ND2	1:A:169:ASP:HB2	2.29	0.47
1:A:116:ASN:H	1:A:116:ASN:HD22	1.62	0.47
1:A:160:ASN:H	1:A:160:ASN:ND2	2.10	0.47
1:A:176:TYR:CB	1:A:177:PHE:CD1	2.97	0.47
1:A:176:TYR:CB	1:A:177:PHE:CE1	2.94	0.47
1:A:49:ILE:HG13	1:A:92:TYR:CB	2.35	0.47
1:A:197:LYS:O	1:A:198:PRO:O	2.30	0.47
1:A:1:THR:HG22	1:A:26:VAL:HG11	1.91	0.47
1:A:38:LYS:C	1:A:40:ASP:H	2.17	0.47
1:B:137:LYS:HG3	1:B:159:ILE:CD1	2.44	0.47
1:B:252:TYR:HE1	1:B:254:LYS:HB2	1.76	0.47
1:B:176:TYR:CB	1:B:177:PHE:CD1	2.97	0.47
1:B:188:PHE:O	1:B:191:TYR:CD2	2.67	0.47
1:B:168:ASN:ND2	1:B:169:ASP:HB2	2.29	0.47
1:A:83:PHE:CB	1:A:84:PRO:HD3	2.42	0.47
1:B:122:GLN:HG3	1:B:136:VAL:HG21	1.96	0.47
1:B:186:GLU:HA	1:B:189:ARG:HG3	1.96	0.47
1:B:222:HIS:CE1	1:B:225:TRP:CZ3	3.02	0.47
1:A:59:ILE:HA	1:A:66:ASN:C	2.34	0.47
1:B:118:ILE:HG22	1:B:118:ILE:O	2.14	0.47
1:B:34:LEU:C	1:B:36:ALA:N	2.67	0.47
1:B:4:THR:HG22	1:B:19:ILE:CA	2.44	0.47
1:B:51:ARG:HG3	1:B:90:HIS:N	2.06	0.47
1:A:129:TYR:CD1	1:A:129:TYR:O	2.67	0.47
1:A:25:PRO:HG3	1:A:257:SER:HA	1.97	0.47
1:B:176:TYR:C	1:B:178:PRO:HD3	2.35	0.47
1:A:176:TYR:C	1:A:178:PRO:HD3	2.35	0.47
1:B:83:PHE:CA	1:B:278:TRP:CD1	2.94	0.47
1:B:89:ILE:O	1:B:89:ILE:HD13	2.14	0.47
1:B:211:LYS:HD3	1:B:212:LYS:HZ3	1.80	0.47
1:A:137:LYS:HE3	1:A:159:ILE:CG2	2.45	0.47
1:A:58:GLU:OE2	1:A:116:ASN:OD1	2.33	0.47
1:B:19:ILE:CD1	1:B:26:VAL:HG13	2.33	0.47
1:A:122:GLN:NE2	1:A:124:GLY:N	2.63	0.47
1:A:144:LEU:O	1:A:151:ASP:HB2	2.14	0.47
1:A:222:HIS:CE1	1:A:225:TRP:CZ3	3.02	0.47
1:B:144:LEU:O	1:B:151:ASP:HB2	2.14	0.47
1:B:176:TYR:CB	1:B:177:PHE:CE1	2.94	0.47
1:B:4:THR:HA	1:B:20:GLU:H	1.80	0.47
1:A:34:LEU:C	1:A:36:ALA:N	2.67	0.47
1:B:137:LYS:HE3	1:B:159:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PRO:CA	1:B:252:TYR:CD2	2.93	0.47
1:B:58:GLU:HG3	1:B:70:GLN:HE22	1.61	0.47
1:A:111:ALA:CB	1:A:145:LEU:HD22	2.44	0.46
1:A:20:GLU:CA	1:A:26:VAL:HG12	2.45	0.46
1:B:116:ASN:HD22	1:B:116:ASN:H	1.62	0.46
1:B:12:THR:CG2	1:B:269:ALA:CB	2.91	0.46
1:B:219:LYS:C	1:B:221:THR:H	2.18	0.46
1:A:186:GLU:HA	1:A:189:ARG:HG3	1.96	0.46
1:A:99:TRP:HZ2	1:A:115:ASN:OD1	1.96	0.46
1:A:247:PRO:CA	1:A:252:TYR:CD2	2.93	0.46
1:A:4:THR:HA	1:A:20:GLU:H	1.80	0.46
1:B:142:MET:HE2	1:B:202:PHE:HZ	1.55	0.46
1:B:59:ILE:HA	1:B:66:ASN:C	2.34	0.46
1:B:57:LEU:HB3	1:B:68:ILE:CA	2.46	0.46
1:A:139:LEU:H	1:A:155:ILE:HG22	1.81	0.46
1:A:161:ASP:OD1	1:A:162:PRO:CD	2.60	0.46
1:A:89:ILE:O	1:A:89:ILE:HD13	2.14	0.46
1:B:122:GLN:NE2	1:B:124:GLY:N	2.63	0.46
1:A:168:ASN:HD22	1:A:168:ASN:C	2.18	0.46
1:A:19:ILE:CD1	1:A:26:VAL:HG13	2.33	0.46
1:B:142:MET:O	1:B:152:TRP:C	2.48	0.46
1:B:20:GLU:CA	1:B:26:VAL:HG12	2.45	0.46
1:A:188:PHE:C	1:A:191:TYR:HB3	2.35	0.46
1:A:4:THR:CG2	1:A:19:ILE:CB	2.94	0.46
1:A:142:MET:HE1	1:A:202:PHE:CZ	2.35	0.46
1:A:29:PHE:HE1	1:A:225:TRP:HD1	1.54	0.46
1:B:106:HIS:CD2	1:B:107:PRO:HD2	2.51	0.46
1:B:71:ASN:O	1:B:72:THR:HB	2.09	0.46
1:A:12:THR:CG2	1:A:269:ALA:CB	2.91	0.46
1:A:54:ASN:CB	1:A:275:ILE:HG21	2.46	0.46
1:B:136:VAL:HG11	1:B:156:ALA:CB	2.36	0.46
1:B:54:ASN:CB	1:B:275:ILE:HG21	2.46	0.46
1:A:10:LYS:N	1:A:15:TYR:CG	2.84	0.46
1:A:54:ASN:CB	1:A:275:ILE:CG2	2.94	0.46
1:B:174:GLU:OE2	1:B:181:LEU:HD12	2.16	0.46
1:B:22:ASP:HB3	1:B:23:GLY:H	1.58	0.46
1:B:38:LYS:C	1:B:40:ASP:H	2.17	0.46
1:B:54:ASN:CB	1:B:275:ILE:CG2	2.94	0.46
1:A:106:HIS:CD2	1:A:107:PRO:HD2	2.51	0.46
1:A:91:ASN:OD1	1:A:128:ALA:HB2	2.16	0.46
1:B:4:THR:CG2	1:B:19:ILE:CB	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:CB	1:B:84:PRO:HD3	2.42	0.46
1:A:118:ILE:O	1:A:118:ILE:HG22	2.14	0.46
1:A:167:LEU:HD11	1:A:177:PHE:HE1	1.81	0.45
1:A:182:ARG:CD	1:A:185:ASP:OD2	2.58	0.45
1:A:219:LYS:C	1:A:221:THR:H	2.18	0.45
1:A:19:ILE:HG23	1:A:26:VAL:HG13	1.99	0.45
1:A:29:PHE:HA	1:A:96:PRO:CB	2.46	0.45
1:B:181:LEU:C	1:B:183:ALA:N	2.66	0.45
1:B:58:GLU:OE2	1:B:116:ASN:OD1	2.33	0.45
1:A:225:TRP:HZ3	1:A:226:LYS:CG	2.13	0.45
1:B:10:LYS:N	1:B:15:TYR:CG	2.84	0.45
1:B:19:ILE:HD13	1:B:26:VAL:HG13	1.75	0.45
1:B:63:GLU:HA	1:B:240:ASP:CG	2.36	0.45
1:A:163:LEU:HD22	1:A:177:PHE:CE1	2.48	0.45
1:B:222:HIS:O	1:B:226:LYS:N	2.47	0.45
1:B:61:LYS:HG3	1:B:239:ILE:CG2	2.47	0.45
1:B:106:HIS:CB	1:B:107:PRO:CD	2.94	0.45
1:A:174:GLU:OE2	1:A:181:LEU:HD12	2.16	0.45
1:A:63:GLU:HA	1:A:240:ASP:CG	2.36	0.45
1:B:25:PRO:HG3	1:B:257:SER:C	2.37	0.45
1:A:10:LYS:CD	1:A:268:ASP:OD2	2.64	0.45
1:A:180:LEU:O	1:A:184:THR:OG1	2.34	0.45
1:A:57:LEU:HB3	1:A:68:ILE:CA	2.46	0.45
1:B:19:ILE:HG23	1:B:26:VAL:HG13	1.99	0.45
1:B:27:SER:O	1:B:31:ASP:HB2	2.16	0.45
1:B:91:ASN:OD1	1:B:128:ALA:HB2	2.16	0.45
1:B:139:LEU:H	1:B:155:ILE:HG22	1.81	0.45
1:A:100:GLU:CG	1:A:117:PRO:O	2.64	0.45
1:A:130:THR:O	1:A:130:THR:HG23	2.15	0.45
1:A:27:SER:O	1:A:31:ASP:HB2	2.16	0.45
1:A:28:ALA:O	1:A:29:PHE:CB	2.63	0.45
1:B:181:LEU:O	1:B:182:ARG:C	2.55	0.45
1:B:9:ALA:HB3	1:B:15:TYR:HA	1.88	0.45
1:A:106:HIS:CB	1:A:107:PRO:CD	2.94	0.45
1:A:146:ASP:O	1:A:147:GLU:C	2.54	0.45
1:B:111:ALA:CB	1:B:145:LEU:CD2	2.94	0.45
1:B:167:LEU:HD11	1:B:177:PHE:HE1	1.81	0.45
1:B:180:LEU:O	1:B:184:THR:OG1	2.34	0.45
1:B:10:LYS:CD	1:B:268:ASP:OD2	2.64	0.45
1:B:19:ILE:C	1:B:26:VAL:CG1	2.85	0.45
1:A:111:ALA:CB	1:A:145:LEU:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:CD	1:A:181:LEU:HD12	2.36	0.45
1:A:25:PRO:HG3	1:A:257:SER:C	2.37	0.45
1:A:4:THR:HA	1:A:20:GLU:N	2.31	0.45
1:B:42:ILE:HG12	1:B:43:PHE:H	0.63	0.45
1:B:65:LEU:O	1:B:66:ASN:CG	2.50	0.45
1:A:225:TRP:CE3	1:A:226:LYS:CA	3.00	0.45
1:B:100:GLU:CG	1:B:117:PRO:O	2.64	0.45
1:B:161:ASP:OD1	1:B:162:PRO:CD	2.60	0.45
1:B:217:ILE:O	1:B:221:THR:HB	2.17	0.45
1:A:177:PHE:O	1:A:179:GLY:N	2.50	0.45
1:A:181:LEU:O	1:A:182:ARG:C	2.55	0.45
1:B:237:LYS:HD3	1:B:241:LEU:HD21	1.99	0.45
1:B:29:PHE:HA	1:B:96:PRO:CB	2.47	0.45
1:A:9:ALA:HB2	1:A:15:TYR:HA	1.98	0.44
1:B:92:TYR:CD2	1:B:121:LEU:HD21	2.51	0.44
1:B:174:GLU:CD	1:B:181:LEU:HD12	2.36	0.44
1:B:190:ILE:HG23	1:B:190:ILE:H	1.56	0.44
1:A:139:LEU:CG	1:A:155:ILE:HG21	2.43	0.44
1:B:168:ASN:HD22	1:B:168:ASN:C	2.18	0.44
1:A:237:LYS:HD3	1:A:241:LEU:HD21	1.99	0.44
1:B:146:ASP:O	1:B:147:GLU:C	2.54	0.44
1:B:47:VAL:HG22	1:B:131:GLY:N	2.26	0.44
1:B:4:THR:HA	1:B:20:GLU:N	2.31	0.44
1:A:12:THR:O	1:A:76:LEU:HD21	2.17	0.44
1:A:84:PRO:O	1:A:85:HIS:HB2	2.12	0.44
1:B:225:TRP:CE3	1:B:226:LYS:CA	3.00	0.44
1:A:71:ASN:O	1:A:72:THR:HB	2.09	0.44
1:A:83:PHE:HA	1:A:278:TRP:CG	2.52	0.44
1:B:134:LYS:CE	1:B:158:ASP:OD1	2.52	0.44
1:B:60:THR:O	1:B:61:LYS:HB2	2.17	0.44
1:A:95:PHE:HD2	1:A:218:ILE:HG12	1.83	0.44
1:A:222:HIS:O	1:A:226:LYS:N	2.47	0.44
1:A:98:THR:CA	1:A:225:TRP:CB	2.96	0.44
1:A:60:THR:O	1:A:61:LYS:HB2	2.17	0.44
1:A:65:LEU:N	1:A:65:LEU:HD22	2.32	0.44
1:B:12:THR:O	1:B:76:LEU:HD21	2.17	0.44
1:A:217:ILE:O	1:A:221:THR:HB	2.17	0.44
1:B:146:ASP:CB	1:B:147:GLU:OE1	2.65	0.44
1:B:42:ILE:HD11	1:B:136:VAL:H	1.83	0.44
1:A:168:ASN:O	1:A:168:ASN:CG	2.56	0.44
1:A:102:PRO:HA	1:A:113:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG11	1:A:156:ALA:CB	2.36	0.44
1:A:146:ASP:CB	1:A:147:GLU:OE1	2.65	0.44
1:A:142:MET:O	1:A:152:TRP:HA	2.18	0.44
1:A:174:GLU:O	1:A:178:PRO:CA	2.57	0.44
1:A:47:VAL:HG22	1:A:131:GLY:N	2.26	0.44
1:A:61:LYS:HG3	1:A:239:ILE:CG2	2.47	0.44
1:B:102:PRO:HA	1:B:113:GLY:C	2.38	0.44
1:B:182:ARG:HA	1:B:182:ARG:HD3	1.72	0.44
1:B:95:PHE:HD2	1:B:218:ILE:HG12	1.83	0.44
1:B:9:ALA:HB2	1:B:15:TYR:HA	1.98	0.44
1:A:6:GLN:O	1:A:265:PRO:N	2.51	0.44
1:A:19:ILE:C	1:A:26:VAL:CG1	2.85	0.44
1:A:27:SER:HB3	1:A:31:ASP:CG	2.39	0.44
1:A:38:LYS:CG	1:A:38:LYS:O	2.66	0.44
1:B:142:MET:O	1:B:152:TRP:HA	2.18	0.44
1:B:177:PHE:O	1:B:179:GLY:N	2.50	0.44
1:B:192:LYS:CE	1:B:200:ASN:HD21	2.29	0.44
1:B:65:LEU:N	1:B:65:LEU:HD22	2.32	0.44
1:B:29:PHE:N	1:B:96:PRO:CB	2.81	0.44
1:A:192:LYS:CE	1:A:200:ASN:HD21	2.29	0.43
1:B:135:GLU:O	1:B:136:VAL:CB	2.38	0.43
1:B:1:THR:H3	1:B:133:VAL:CG1	2.25	0.43
1:B:6:GLN:O	1:B:265:PRO:N	2.51	0.43
1:A:143:ALA:O	1:A:202:PHE:HD1	1.99	0.43
1:A:58:GLU:HG3	1:A:70:GLN:HE22	1.62	0.43
1:A:52:TRP:HB3	1:A:86:HIS:CD2	2.53	0.43
1:B:80:ARG:HG3	1:B:194:PRO:CG	2.48	0.43
1:B:193:ILE:H	1:B:193:ILE:HG12	1.55	0.43
1:A:98:THR:HG22	1:A:99:TRP:N	2.33	0.43
1:B:188:PHE:C	1:B:191:TYR:HB3	2.35	0.43
1:B:98:THR:CA	1:B:225:TRP:CB	2.96	0.43
1:B:27:SER:HB3	1:B:31:ASP:CG	2.38	0.43
1:B:62:GLU:O	1:B:63:GLU:CB	2.44	0.43
1:B:57:LEU:CB	1:B:68:ILE:H	2.31	0.43
1:A:163:LEU:HB3	1:A:167:LEU:CD1	2.49	0.43
1:A:182:ARG:HD3	1:A:182:ARG:HA	1.72	0.43
1:A:42:ILE:HD11	1:A:136:VAL:H	1.83	0.43
1:A:83:PHE:CZ	1:B:179:GLY:HA3	2.53	0.43
1:B:52:TRP:HB3	1:B:86:HIS:CD2	2.53	0.43
1:B:209:LYS:HB2	1:B:213:TYR:CB	2.49	0.43
1:B:232:LYS:O	1:B:234:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:O	1:A:152:TRP:C	2.48	0.43
1:A:170:ILE:CG1	1:A:210:ASN:HA	2.48	0.43
1:A:179:GLY:HA3	1:B:83:PHE:CZ	2.53	0.43
1:A:209:LYS:HB2	1:A:213:TYR:CB	2.49	0.43
1:A:51:ARG:HG3	1:A:90:HIS:N	2.06	0.43
1:A:95:PHE:HD2	1:A:218:ILE:CG1	2.32	0.43
1:B:81:ASN:OD1	1:B:87:GLY:N	2.51	0.43
1:A:83:PHE:CE1	1:A:280:PHE:CZ	2.98	0.43
1:A:81:ASN:OD1	1:A:87:GLY:N	2.51	0.43
1:A:8:GLY:HA3	1:A:266:LYS:N	2.34	0.43
1:B:238:GLY:O	1:B:239:ILE:CG2	2.56	0.43
1:B:168:ASN:O	1:B:168:ASN:CG	2.56	0.43
1:A:105:SER:HB2	1:A:112:VAL:CA	2.24	0.43
1:A:215:LEU:O	1:A:219:LYS:HB2	2.19	0.43
1:B:176:TYR:C	1:B:178:PRO:CD	2.88	0.43
1:B:215:LEU:O	1:B:219:LYS:HB2	2.19	0.43
1:A:176:TYR:C	1:A:178:PRO:CD	2.87	0.42
1:A:232:LYS:O	1:A:234:SER:N	2.51	0.42
1:B:111:ALA:O	1:B:112:VAL:C	2.57	0.42
1:B:170:ILE:CG1	1:B:210:ASN:HA	2.48	0.42
1:B:174:GLU:O	1:B:178:PRO:CA	2.57	0.42
1:B:34:LEU:HD21	1:B:95:PHE:CA	2.49	0.42
1:B:95:PHE:HD2	1:B:218:ILE:CG1	2.32	0.42
1:B:98:THR:HG22	1:B:99:TRP:N	2.33	0.42
1:A:238:GLY:O	1:A:239:ILE:CG2	2.56	0.42
1:A:29:PHE:N	1:A:96:PRO:CB	2.81	0.42
1:A:34:LEU:HD21	1:A:95:PHE:CA	2.49	0.42
1:A:36:ALA:O	1:A:43:PHE:HA	2.19	0.42
1:A:57:LEU:CB	1:A:68:ILE:H	2.31	0.42
1:B:142:MET:HB3	1:B:153:LYS:CG	2.50	0.42
1:B:182:ARG:CD	1:B:185:ASP:OD2	2.58	0.42
1:B:244:VAL:CG2	1:B:254:LYS:HG3	2.49	0.42
1:A:117:PRO:HB2	1:A:118:ILE:H	1.67	0.42
1:A:179:GLY:C	1:B:83:PHE:HZ	2.22	0.42
1:A:30:HIS:CD2	1:A:241:LEU:O	2.72	0.42
1:A:83:PHE:HZ	1:B:179:GLY:C	2.22	0.42
1:B:30:HIS:CD2	1:B:241:LEU:O	2.72	0.42
1:B:95:PHE:CD2	1:B:218:ILE:CG1	3.02	0.42
1:A:111:ALA:O	1:A:112:VAL:C	2.57	0.42
1:A:226:LYS:O	1:A:228:LEU:N	2.53	0.42
1:A:69:ILE:CG2	1:A:77:ARG:H	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HG3	1:A:194:PRO:CG	2.48	0.42
1:B:142:MET:HB3	1:B:153:LYS:HG2	2.01	0.42
1:B:8:GLY:HA3	1:B:266:LYS:N	2.34	0.42
1:A:142:MET:HB3	1:A:153:LYS:CG	2.50	0.42
1:B:105:SER:H	1:B:112:VAL:CG1	2.20	0.42
1:A:277:LYS:HG2	1:B:125:GLU:OE2	2.10	0.42
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.84	0.42
1:B:226:LYS:O	1:B:228:LEU:N	2.53	0.42
1:A:118:ILE:HD12	1:A:221:THR:CB	2.49	0.42
1:A:125:GLU:OE2	1:B:277:LYS:HG2	2.10	0.42
1:A:164:ALA:O	1:A:166:LYS:N	2.53	0.42
1:A:19:ILE:HD13	1:A:26:VAL:HG13	1.75	0.42
1:B:36:ALA:O	1:B:43:PHE:HA	2.19	0.42
1:B:83:PHE:HA	1:B:278:TRP:CG	2.52	0.42
1:A:134:LYS:CE	1:A:158:ASP:OD1	2.52	0.42
1:A:95:PHE:CD2	1:A:218:ILE:CG1	3.02	0.42
1:B:252:TYR:C	1:B:252:TYR:CD1	2.92	0.42
1:A:42:ILE:CB	1:A:159:ILE:HD11	2.50	0.42
1:A:136:VAL:C	1:A:159:ILE:HG13	2.40	0.42
1:A:244:VAL:CG2	1:A:254:LYS:HG3	2.49	0.42
1:A:9:ALA:HB3	1:A:15:TYR:HA	1.88	0.42
1:B:136:VAL:HG22	1:B:157:ILE:H	1.14	0.42
1:B:41:ASN:HB3	1:B:42:ILE:H	1.72	0.42
1:A:177:PHE:HD1	1:A:177:PHE:H	1.68	0.42
1:A:59:ILE:HG13	1:A:65:LEU:HB3	2.02	0.42
1:B:10:LYS:O	1:B:11:ASN:ND2	2.53	0.42
1:B:118:ILE:HD12	1:B:221:THR:CB	2.49	0.42
1:B:214:ALA:O	1:B:218:ILE:N	2.41	0.42
1:B:59:ILE:HB	1:B:66:ASN:CA	2.49	0.42
1:A:241:LEU:N	1:A:241:LEU:CD1	2.83	0.42
1:A:252:TYR:C	1:A:252:TYR:CD1	2.92	0.42
1:A:275:ILE:O	1:A:277:LYS:CB	2.66	0.42
1:A:59:ILE:HB	1:A:66:ASN:CA	2.49	0.42
1:A:10:LYS:C	1:A:11:ASN:CG	2.77	0.41
1:A:7:ILE:C	1:A:8:GLY:O	2.50	0.41
1:B:136:VAL:C	1:B:159:ILE:HG13	2.40	0.41
1:B:25:PRO:HG3	1:B:257:SER:HA	1.97	0.41
1:B:38:LYS:CG	1:B:38:LYS:O	2.66	0.41
1:A:16:LYS:HE2	1:A:62:GLU:OE2	2.20	0.41
1:A:45:MET:HB3	1:A:95:PHE:HE1	1.86	0.41
1:B:122:GLN:HG2	1:B:156:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LYS:HE2	1:B:62:GLU:OE2	2.20	0.41
1:B:200:ASN:HA	1:B:200:ASN:HD22	1.60	0.41
1:B:32:ILE:HG21	1:B:96:PRO:HG3	2.00	0.41
1:A:10:LYS:O	1:A:11:ASN:ND2	2.53	0.41
1:A:122:GLN:HG2	1:A:156:ALA:O	2.20	0.41
1:A:42:ILE:CD1	1:A:136:VAL:H	2.33	0.41
1:A:148:GLY:O	1:A:149:GLU:HG2	2.20	0.41
1:A:41:ASN:HB3	1:A:42:ILE:H	1.72	0.41
1:B:42:ILE:CB	1:B:159:ILE:HD11	2.50	0.41
1:B:218:ILE:O	1:B:218:ILE:HG23	2.17	0.41
1:B:34:LEU:C	1:B:43:PHE:CB	2.82	0.41
1:A:139:LEU:N	1:A:155:ILE:HG22	2.36	0.41
1:A:142:MET:HB3	1:A:153:LYS:HG2	2.01	0.41
1:A:175:LYS:C	1:A:178:PRO:HD3	2.41	0.41
1:A:193:ILE:HG12	1:A:193:ILE:H	1.55	0.41
1:B:112:VAL:HB	1:B:113:GLY:H	1.51	0.41
1:B:42:ILE:CD1	1:B:136:VAL:H	2.33	0.41
1:B:113:GLY:HA2	1:B:150:THR:HB	2.02	0.41
1:B:160:ASN:HD22	1:B:161:ASP:H	1.67	0.41
1:B:164:ALA:O	1:B:166:LYS:N	2.53	0.41
1:B:225:TRP:CE3	1:B:226:LYS:HA	2.55	0.41
1:B:275:ILE:O	1:B:277:LYS:CB	2.66	0.41
1:B:64:THR:O	1:B:65:LEU:HD22	2.20	0.41
1:B:139:LEU:N	1:B:155:ILE:HG22	2.36	0.41
1:A:113:GLY:HA2	1:A:150:THR:HB	2.03	0.41
1:A:242:THR:HA	1:A:251:THR:O	2.20	0.41
1:A:28:ALA:HA	1:A:32:ILE:CG1	2.48	0.41
1:B:147:GLU:N	1:B:147:GLU:OE1	2.54	0.41
1:B:163:LEU:HB3	1:B:167:LEU:CD1	2.49	0.41
1:B:189:ARG:C	1:B:191:TYR:N	2.74	0.41
1:B:191:TYR:CD2	1:B:192:LYS:N	2.89	0.41
1:A:177:PHE:CA	1:B:280:PHE:CE2	3.03	0.41
1:A:225:TRP:CE3	1:A:226:LYS:HA	2.55	0.41
1:A:249:THR:C	1:A:251:THR:N	2.59	0.41
1:A:81:ASN:O	1:A:278:TRP:HD1	2.04	0.41
1:B:134:LYS:HE3	1:B:158:ASP:CG	2.37	0.41
1:A:92:TYR:CD2	1:A:121:LEU:HD21	2.51	0.41
1:A:142:MET:CE	1:A:202:PHE:HE1	2.16	0.41
1:A:228:LEU:O	1:A:229:ILE:C	2.59	0.41
1:B:242:THR:HA	1:B:251:THR:O	2.20	0.41
1:A:200:ASN:C	1:A:201:GLN:CG	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:O	1:A:218:ILE:HG23	2.17	0.41
1:B:148:GLY:O	1:B:149:GLU:HG2	2.20	0.41
1:B:182:ARG:NH1	1:B:185:ASP:CB	2.66	0.41
1:B:139:LEU:O	1:B:211:LYS:HB2	2.21	0.41
1:A:112:VAL:O	1:A:150:THR:CG2	2.61	0.41
1:A:147:GLU:N	1:A:147:GLU:OE1	2.54	0.41
1:A:191:TYR:CD2	1:A:192:LYS:N	2.89	0.41
1:B:65:LEU:C	1:B:66:ASN:ND2	2.63	0.41
1:A:4:THR:HA	1:A:19:ILE:HA	2.03	0.41
1:A:59:ILE:CG2	1:A:67:PRO:CD	2.96	0.41
1:B:192:LYS:O	1:B:193:ILE:O	2.39	0.41
1:B:64:THR:O	1:B:65:LEU:CD2	2.69	0.41
1:A:193:ILE:CB	1:A:194:PRO:HD2	2.46	0.41
1:A:214:ALA:O	1:A:218:ILE:N	2.41	0.41
1:A:34:LEU:C	1:A:43:PHE:CB	2.82	0.41
1:A:51:ARG:CG	1:A:89:ILE:HA	2.19	0.41
1:A:92:TYR:HD2	1:A:121:LEU:CD2	2.25	0.41
1:A:33:PRO:O	1:A:97:GLN:HG3	2.21	0.41
1:B:141:ILE:CA	1:B:153:LYS:O	2.67	0.41
1:B:175:LYS:C	1:B:178:PRO:HD3	2.41	0.41
1:B:193:ILE:CB	1:B:194:PRO:HD2	2.46	0.41
1:B:59:ILE:HG22	1:B:67:PRO:HA	1.93	0.41
1:B:59:ILE:HG13	1:B:65:LEU:HB3	2.02	0.41
1:A:50:PRO:HB3	1:A:128:ALA:CB	2.29	0.40
1:A:64:THR:O	1:A:65:LEU:CD2	2.69	0.40
1:B:130:THR:HG23	1:B:130:THR:O	2.15	0.40
1:B:129:TYR:HD2	1:B:132:GLN:CD	2.25	0.40
1:B:137:LYS:CG	1:B:159:ILE:CD1	3.00	0.40
1:B:5:ARG:HH22	1:B:25:PRO:CG	2.35	0.40
1:B:81:ASN:HD21	1:B:86:HIS:CE1	2.39	0.40
1:A:170:ILE:HG13	1:A:210:ASN:HA	2.03	0.40
1:A:234:SER:HB2	1:A:237:LYS:HG3	2.03	0.40
1:B:173:VAL:HA	1:B:177:PHE:CD1	2.55	0.40
1:B:4:THR:HA	1:B:19:ILE:HA	2.03	0.40
1:B:217:ILE:HD12	1:B:220:GLU:CD	2.42	0.40
1:A:139:LEU:O	1:A:211:LYS:HB2	2.21	0.40
1:A:80:ARG:HD3	1:A:279:PHE:HD1	1.84	0.40
1:A:83:PHE:N	1:A:84:PRO:HD2	2.37	0.40
1:B:102:PRO:O	1:B:112:VAL:CB	2.63	0.40
1:B:177:PHE:HD1	1:B:177:PHE:H	1.68	0.40
1:B:83:PHE:N	1:B:84:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:O	1:B:97:GLN:HG3	2.21	0.40
1:A:190:ILE:HG23	1:A:190:ILE:H	1.56	0.40
1:A:22:ASP:HB3	1:A:23:GLY:H	1.58	0.40
1:A:32:ILE:HG21	1:A:96:PRO:HG3	2.00	0.40
1:B:80:ARG:HG2	1:B:194:PRO:O	2.21	0.40
1:B:51:ARG:CG	1:B:89:ILE:HA	2.19	0.40
1:A:111:ALA:C	1:A:112:VAL:HG23	2.42	0.40
1:A:219:LYS:C	1:A:221:THR:N	2.75	0.40
1:B:82:CYS:HB3	1:B:190:ILE:CD1	2.52	0.40
1:B:234:SER:HB2	1:B:237:LYS:HG3	2.04	0.40
1:B:59:ILE:CG2	1:B:67:PRO:CD	2.96	0.40
1:B:81:ASN:O	1:B:278:TRP:HD1	2.04	0.40
1:B:45:MET:HB3	1:B:95:PHE:HE1	1.86	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:CG	1:B:108:GLU:OE2[1_445]	1.56	0.64
1:A:115:ASN:ND2	1:B:75:LYS:NZ[1_455]	1.71	0.49
1:A:174:GLU:OE1	1:B:248:ASP:CG[2_775]	1.72	0.48
1:B:2:TYR:OH	1:B:199:GLU:OE2[2_774]	1.82	0.38
1:A:247:PRO:CG	1:B:108:GLU:CG[1_445]	1.84	0.36
1:A:174:GLU:OE1	1:B:248:ASP:OD1[2_775]	1.85	0.35
1:A:147:GLU:O	1:B:73:LYS:NZ[1_455]	1.85	0.35
1:B:24:LYS:NZ	1:B:182:ARG:NE[2_774]	1.92	0.28
1:B:24:LYS:CE	1:B:182:ARG:NH2[2_774]	1.95	0.25
1:A:247:PRO:CG	1:B:108:GLU:CD[1_445]	2.05	0.15
1:A:252:TYR:OH	1:B:106:HIS:CD2[1_445]	2.07	0.13
1:A:174:GLU:OE1	1:B:248:ASP:OD2[2_775]	2.15	0.05
1:A:149:GLU:CG	1:B:73:LYS:NZ[1_455]	2.18	0.02

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	279/285 (98%)	151 (54%)	53 (19%)	75 (27%)	0	0
1	B	279/285 (98%)	152 (54%)	53 (19%)	74 (26%)	0	0
All	All	558/570 (98%)	303 (54%)	106 (19%)	149 (27%)	0	0

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	8	GLY
1	A	9	ALA
1	A	12	THR
1	A	13	LEU
1	A	24	LYS
1	A	33	PRO
1	A	37	ASP
1	A	39	GLU
1	A	63	GLU
1	A	70	GLN
1	A	82	CYS
1	A	85	HIS
1	A	91	ASN
1	A	94	ALA
1	A	104	VAL
1	A	111	ALA
1	A	116	ASN
1	A	117	PRO
1	A	130	THR
1	A	136	VAL
1	A	159	ILE
1	A	172	ASP
1	A	173	VAL
1	A	181	LEU
1	A	185	ASP
1	A	186	GLU
1	A	187	TRP
1	A	193	ILE
1	A	195	ASP
1	A	198	PRO
1	A	201	GLN
1	A	205	SER

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Mol	Chain	Res	Type
1	A	233	SER
1	A	275	ILE
1	A	276	ASP
1	B	2	TYR
1	B	8	GLY
1	B	9	ALA
1	B	12	THR
1	B	13	LEU
1	B	24	LYS
1	B	33	PRO
1	B	37	ASP
1	B	39	GLU
1	B	63	GLU
1	B	70	GLN
1	B	82	CYS
1	B	85	HIS
1	B	91	ASN
1	B	94	ALA
1	B	104	VAL
1	B	111	ALA
1	B	116	ASN
1	B	117	PRO
1	B	130	THR
1	B	136	VAL
1	B	159	ILE
1	B	172	ASP
1	B	173	VAL
1	B	181	LEU
1	B	185	ASP
1	B	186	GLU
1	B	187	TRP
1	B	193	ILE
1	B	195	ASP
1	B	198	PRO
1	B	201	GLN
1	B	205	SER
1	B	233	SER
1	B	275	ILE
1	B	276	ASP
1	A	10	LYS
1	A	11	ASN
1	A	26	VAL

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Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	TYR
1	A	62	GLU
1	A	72	THR
1	A	75	LYS
1	A	90	HIS
1	A	92	TYR
1	A	97	GLN
1	A	108	GLU
1	A	182	ARG
1	A	230	ALA
1	A	239	ILE
1	A	242	THR
1	A	254	LYS
1	B	10	LYS
1	B	11	ASN
1	B	26	VAL
1	B	34	LEU
1	B	35	TYR
1	B	62	GLU
1	B	72	THR
1	B	75	LYS
1	B	90	HIS
1	B	92	TYR
1	B	97	GLN
1	B	108	GLU
1	B	182	ARG
1	B	230	ALA
1	B	239	ILE
1	B	242	THR
1	B	254	LYS
1	A	42	ILE
1	A	112	VAL
1	A	171	GLU
1	B	42	ILE
1	B	112	VAL
1	B	171	GLU
1	A	25	PRO
1	A	74	GLY
1	A	95	PHE
1	A	148	GLY
1	A	164	ALA

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Mol	Chain	Res	Type
1	A	204	PHE
1	A	247	PRO
1	B	25	PRO
1	B	74	GLY
1	B	95	PHE
1	B	148	GLY
1	B	164	ALA
1	B	204	PHE
1	B	247	PRO
1	A	65	LEU
1	A	194	PRO
1	A	203	ALA
1	A	250	PRO
1	B	65	LEU
1	B	194	PRO
1	B	203	ALA
1	B	250	PRO
1	A	15	TYR
1	A	49	ILE
1	A	68	ILE
1	A	105	SER
1	A	178	PRO
1	B	15	TYR
1	B	49	ILE
1	B	68	ILE
1	B	178	PRO
1	A	127	ILE
1	B	127	ILE
1	A	59	ILE
1	B	59	ILE
1	A	83	PHE
1	B	83	PHE

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	243/247 (98%)	158 (65%)	85 (35%)	0	1
1	B	243/247 (98%)	158 (65%)	85 (35%)	0	1
All	All	486/494 (98%)	316 (65%)	170 (35%)	0	1

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	ILE
1	A	17	VAL
1	A	19	ILE
1	A	26	VAL
1	A	27	SER
1	A	35	TYR
1	A	40	ASP
1	A	41	ASN
1	A	42	ILE
1	A	43	PHE
1	A	44	ASN
1	A	45	MET
1	A	48	GLU
1	A	49	ILE
1	A	51	ARG
1	A	53	THR
1	A	54	ASN
1	A	57	LEU
1	A	60	THR
1	A	62	GLU
1	A	63	GLU
1	A	65	LEU
1	A	66	ASN
1	A	79	VAL
1	A	80	ARG
1	A	83	PHE
1	A	86	HIS
1	A	89	ILE
1	A	92	TYR
1	A	99	TRP
1	A	100	GLU
1	A	104	VAL
1	A	106	HIS
1	A	109	THR

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	115	ASN
1	A	118	ILE
1	A	121	LEU
1	A	123	ILE
1	A	125	GLU
1	A	126	THR
1	A	130	THR
1	A	135	GLU
1	A	136	VAL
1	A	141	ILE
1	A	144	LEU
1	A	150	THR
1	A	151	ASP
1	A	153	LYS
1	A	155	ILE
1	A	158	ASP
1	A	160	ASN
1	A	161	ASP
1	A	163	LEU
1	A	168	ASN
1	A	169	ASP
1	A	171	GLU
1	A	177	PHE
1	A	182	ARG
1	A	187	TRP
1	A	189	ARG
1	A	191	TYR
1	A	193	ILE
1	A	200	ASN
1	A	210	ASN
1	A	211	LYS
1	A	212	LYS
1	A	213	TYR
1	A	217	ILE
1	A	218	ILE
1	A	220	GLU
1	A	223	ASN
1	A	224	SER
1	A	225	TRP
1	A	229	ILE
1	A	239	ILE

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Mol	Chain	Res	Type
1	A	240	ASP
1	A	242	THR
1	A	251	THR
1	A	258	ASP
1	A	271	ILE
1	A	272	ASP
1	A	276	ASP
1	A	278	TRP
1	B	3	THR
1	B	7	ILE
1	B	17	VAL
1	B	19	ILE
1	B	26	VAL
1	B	27	SER
1	B	35	TYR
1	B	40	ASP
1	B	41	ASN
1	B	42	ILE
1	B	43	PHE
1	B	44	ASN
1	B	45	MET
1	B	48	GLU
1	B	49	ILE
1	B	51	ARG
1	B	53	THR
1	B	54	ASN
1	B	57	LEU
1	B	60	THR
1	B	62	GLU
1	B	63	GLU
1	B	65	LEU
1	B	66	ASN
1	B	79	VAL
1	B	80	ARG
1	B	83	PHE
1	B	86	HIS
1	B	89	ILE
1	B	92	TYR
1	B	99	TRP
1	B	100	GLU
1	B	104	VAL
1	B	106	HIS

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Mol	Chain	Res	Type
1	B	109	THR
1	B	112	VAL
1	B	115	ASN
1	B	118	ILE
1	B	121	LEU
1	B	123	ILE
1	B	125	GLU
1	B	126	THR
1	B	130	THR
1	B	135	GLU
1	B	136	VAL
1	B	141	ILE
1	B	144	LEU
1	B	150	THR
1	B	151	ASP
1	B	153	LYS
1	B	155	ILE
1	B	158	ASP
1	B	160	ASN
1	B	161	ASP
1	B	163	LEU
1	B	168	ASN
1	B	169	ASP
1	B	171	GLU
1	B	177	PHE
1	B	182	ARG
1	B	187	TRP
1	B	189	ARG
1	B	191	TYR
1	B	193	ILE
1	B	200	ASN
1	B	210	ASN
1	B	211	LYS
1	B	212	LYS
1	B	213	TYR
1	B	217	ILE
1	B	218	ILE
1	B	220	GLU
1	B	223	ASN
1	B	224	SER
1	B	225	TRP
1	B	229	ILE

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Mol	Chain	Res	Type
1	B	239	ILE
1	B	240	ASP
1	B	242	THR
1	B	251	THR
1	B	258	ASP
1	B	271	ILE
1	B	272	ASP
1	B	276	ASP
1	B	278	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	66	ASN
1	A	122	GLN
1	A	160	ASN
1	A	168	ASN
1	A	200	ASN
1	B	41	ASN
1	B	66	ASN
1	B	122	GLN
1	B	160	ASN
1	B	168	ASN
1	B	200	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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.