



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:19 PM UTC

PDB ID : 9MLH / pdb_00009mlh
EMDB ID : EMD-48372
Title : Xenorhabdus nematophilus XptA2, wild type State 2
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

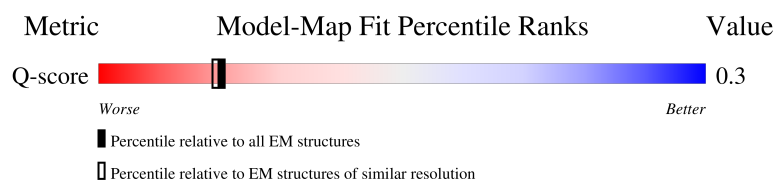
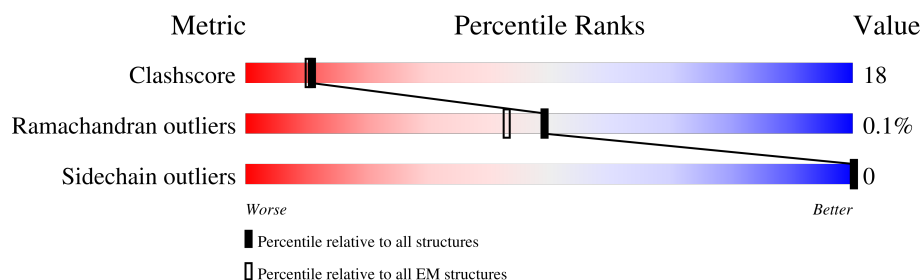
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2538	
1	B	2538	
1	C	2538	
1	D	2538	

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Mol	Chain	Length	Quality of chain
1	E	2538	 A horizontal bar chart showing the quality of chain E. The bar is divided into two segments: a green segment on the left representing 64% and a yellow segment on the right representing 35%. A small red dot is visible at the beginning of the green segment.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 XptA2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2537	Total 20006	C 12625	N 3414	O 3894	S 73	0	0
1	B	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	C	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	D	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	E	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0

There are 605 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	HIS	PRO	conflict	UNP Q93RN7
A	343	ASN	HIS	conflict	UNP Q93RN7
A	344	ILE	VAL	conflict	UNP Q93RN7
A	360	ARG	CYS	conflict	UNP Q93RN7
A	365	VAL	ILE	conflict	UNP Q93RN7
A	377	ALA	SER	conflict	UNP Q93RN7
A	379	PRO	THR	conflict	UNP Q93RN7
A	391	ILE	VAL	conflict	UNP Q93RN7
A	407	SER	ASN	conflict	UNP Q93RN7
A	410	LYS	ARG	conflict	UNP Q93RN7
A	566	VAL	ILE	conflict	UNP Q93RN7
A	583	ALA	THR	conflict	UNP Q93RN7
A	586	THR	ILE	conflict	UNP Q93RN7
A	587	ILE	LEU	conflict	UNP Q93RN7
A	592	PHE	PRO	conflict	UNP Q93RN7
A	606	VAL	ALA	conflict	UNP Q93RN7
A	620	LEU	PHE	conflict	UNP Q93RN7
A	637	PRO	SER	conflict	UNP Q93RN7
A	682	ASN	THR	conflict	UNP Q93RN7
A	686	SER	ARG	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	695	HIS	SER	conflict	UNP Q93RN7
A	696	ASN	ASP	conflict	UNP Q93RN7
A	736	ASP	ASN	conflict	UNP Q93RN7
A	742	THR	MET	conflict	UNP Q93RN7
A	748	SER	THR	conflict	UNP Q93RN7
A	750	ASN	SER	conflict	UNP Q93RN7
A	751	ALA	ASP	conflict	UNP Q93RN7
A	752	ASN	GLU	conflict	UNP Q93RN7
A	788	GLY	ASP	conflict	UNP Q93RN7
A	790	ALA	VAL	conflict	UNP Q93RN7
A	795	LYS	ARG	conflict	UNP Q93RN7
A	796	ASN	SER	conflict	UNP Q93RN7
A	799	ALA	PRO	conflict	UNP Q93RN7
A	800	GLY	ASP	conflict	UNP Q93RN7
A	801	GLN	ASN	conflict	UNP Q93RN7
A	?	-	THR	deletion	UNP Q93RN7
A	?	-	ILE	deletion	UNP Q93RN7
A	?	-	LEU	deletion	UNP Q93RN7
A	?	-	ILE	deletion	UNP Q93RN7
A	?	-	LEU	deletion	UNP Q93RN7
A	?	-	CYS	deletion	UNP Q93RN7
A	?	-	SER	deletion	UNP Q93RN7
A	803	ASN	SER	conflict	UNP Q93RN7
A	804	ILE	THR	conflict	UNP Q93RN7
A	806	THR	SER	conflict	UNP Q93RN7
A	807	LEU	THR	conflict	UNP Q93RN7
A	808	PHE	SER	conflict	UNP Q93RN7
A	809	SER	GLY	conflict	UNP Q93RN7
A	811	TYR	MET	conflict	UNP Q93RN7
A	812	ARG	-	insertion	UNP Q93RN7
A	813	PHE	-	insertion	UNP Q93RN7
A	814	HIS	-	insertion	UNP Q93RN7
A	815	GLN	-	insertion	UNP Q93RN7
A	816	TRP	-	insertion	UNP Q93RN7
A	817	ILE	-	insertion	UNP Q93RN7
A	818	ASN	-	insertion	UNP Q93RN7
A	820	LEU	TRP	conflict	UNP Q93RN7
A	821	GLY	GLU	conflict	UNP Q93RN7
A	822	ASN	ILE	conflict	UNP Q93RN7
A	824	GLY	ALA	conflict	UNP Q93RN7
A	825	SER	LEU	conflict	UNP Q93RN7
A	826	ASP	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	827	THR	ARG	conflict	UNP Q93RN7
A	828	LEU	TRP	conflict	UNP Q93RN7
A	829	ASP	ILE	conflict	UNP Q93RN7
A	830	MET	CYS	conflict	UNP Q93RN7
A	831	LEU	CYS	conflict	UNP Q93RN7
A	832	ARG	ALA	conflict	UNP Q93RN7
A	833	GLN	LYS	conflict	UNP Q93RN7
A	838	ALA	GLY	conflict	UNP Q93RN7
A	842	ALA	GLY	conflict	UNP Q93RN7
A	843	SER	LEU	conflict	UNP Q93RN7
A	844	VAL	ARG	conflict	UNP Q93RN7
A	845	MET	ASP	conflict	UNP Q93RN7
A	847	LEU	ALA	conflict	UNP Q93RN7
A	848	ASP	GLY	conflict	UNP Q93RN7
A	849	ILE	HIS	conflict	UNP Q93RN7
A	850	SER	GLN	conflict	UNP Q93RN7
A	851	MET	TYR	conflict	UNP Q93RN7
A	852	VAL	GLY	conflict	UNP Q93RN7
A	853	THR	ASN	conflict	UNP Q93RN7
A	854	GLN	ALA	conflict	UNP Q93RN7
A	855	ALA	GLY	conflict	UNP Q93RN7
A	856	MET	HIS	conflict	UNP Q93RN7
A	857	VAL	GLY	conflict	UNP Q93RN7
A	872	THR	PRO	conflict	UNP Q93RN7
A	878	ASP	HIS	conflict	UNP Q93RN7
A	884	HIS	ILE	conflict	UNP Q93RN7
A	911	SER	ALA	conflict	UNP Q93RN7
A	914	GLU	LYS	conflict	UNP Q93RN7
A	923	GLU	ALA	conflict	UNP Q93RN7
A	1067	LYS	GLN	conflict	UNP Q93RN7
A	1075	ASP	GLU	conflict	UNP Q93RN7
A	1126	ASP	ASN	conflict	UNP Q93RN7
A	1250	LYS	VAL	conflict	UNP Q93RN7
A	1253	SER	PRO	conflict	UNP Q93RN7
A	1257	GLY	ASP	conflict	UNP Q93RN7
A	1258	SER	ASN	conflict	UNP Q93RN7
A	1514	ILE	VAL	conflict	UNP Q93RN7
A	1519	MET	VAL	conflict	UNP Q93RN7
A	1877	ASN	TYR	conflict	UNP Q93RN7
A	1880	MET	THR	conflict	UNP Q93RN7
A	1884	ILE	VAL	conflict	UNP Q93RN7
A	1920	THR	ALA	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1943	GLY	VAL	conflict	UNP Q93RN7
A	1947	GLN	HIS	conflict	UNP Q93RN7
A	1959	MET	ALA	conflict	UNP Q93RN7
A	1961	GLY	ASP	conflict	UNP Q93RN7
A	1962	ARG	ASN	conflict	UNP Q93RN7
A	1964	GLY	GLU	conflict	UNP Q93RN7
A	1966	SER	ALA	conflict	UNP Q93RN7
A	1967	LYS	THR	conflict	UNP Q93RN7
A	1968	ASN	GLN	conflict	UNP Q93RN7
A	1969	LEU	PRO	conflict	UNP Q93RN7
A	2028	THR	PRO	conflict	UNP Q93RN7
A	2057	THR	ALA	conflict	UNP Q93RN7
A	2149	LEU	PHE	conflict	UNP Q93RN7
A	2161	VAL	ALA	conflict	UNP Q93RN7
A	2164	ILE	VAL	conflict	UNP Q93RN7
A	2178	LEU	PHE	conflict	UNP Q93RN7
A	2430	LEU	PHE	conflict	UNP Q93RN7
B	172	HIS	PRO	conflict	UNP Q93RN7
B	343	ASN	HIS	conflict	UNP Q93RN7
B	344	ILE	VAL	conflict	UNP Q93RN7
B	360	ARG	CYS	conflict	UNP Q93RN7
B	365	VAL	ILE	conflict	UNP Q93RN7
B	377	ALA	SER	conflict	UNP Q93RN7
B	379	PRO	THR	conflict	UNP Q93RN7
B	391	ILE	VAL	conflict	UNP Q93RN7
B	407	SER	ASN	conflict	UNP Q93RN7
B	410	LYS	ARG	conflict	UNP Q93RN7
B	566	VAL	ILE	conflict	UNP Q93RN7
B	583	ALA	THR	conflict	UNP Q93RN7
B	586	THR	ILE	conflict	UNP Q93RN7
B	587	ILE	LEU	conflict	UNP Q93RN7
B	592	PHE	PRO	conflict	UNP Q93RN7
B	606	VAL	ALA	conflict	UNP Q93RN7
B	620	LEU	PHE	conflict	UNP Q93RN7
B	637	PRO	SER	conflict	UNP Q93RN7
B	682	ASN	THR	conflict	UNP Q93RN7
B	686	SER	ARG	conflict	UNP Q93RN7
B	695	HIS	SER	conflict	UNP Q93RN7
B	696	ASN	ASP	conflict	UNP Q93RN7
B	736	ASP	ASN	conflict	UNP Q93RN7
B	742	THR	MET	conflict	UNP Q93RN7
B	748	SER	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	750	ASN	SER	conflict	UNP Q93RN7
B	751	ALA	ASP	conflict	UNP Q93RN7
B	752	ASN	GLU	conflict	UNP Q93RN7
B	788	GLY	ASP	conflict	UNP Q93RN7
B	790	ALA	VAL	conflict	UNP Q93RN7
B	795	LYS	ARG	conflict	UNP Q93RN7
B	796	ASN	SER	conflict	UNP Q93RN7
B	799	ALA	PRO	conflict	UNP Q93RN7
B	800	GLY	ASP	conflict	UNP Q93RN7
B	801	GLN	ASN	conflict	UNP Q93RN7
B	?	-	THR	deletion	UNP Q93RN7
B	?	-	ILE	deletion	UNP Q93RN7
B	?	-	LEU	deletion	UNP Q93RN7
B	?	-	ILE	deletion	UNP Q93RN7
B	?	-	LEU	deletion	UNP Q93RN7
B	?	-	CYS	deletion	UNP Q93RN7
B	?	-	SER	deletion	UNP Q93RN7
B	803	ASN	SER	conflict	UNP Q93RN7
B	804	ILE	THR	conflict	UNP Q93RN7
B	806	THR	SER	conflict	UNP Q93RN7
B	807	LEU	THR	conflict	UNP Q93RN7
B	808	PHE	SER	conflict	UNP Q93RN7
B	809	SER	GLY	conflict	UNP Q93RN7
B	811	TYR	MET	conflict	UNP Q93RN7
B	812	ARG	-	insertion	UNP Q93RN7
B	813	PHE	-	insertion	UNP Q93RN7
B	814	HIS	-	insertion	UNP Q93RN7
B	815	GLN	-	insertion	UNP Q93RN7
B	816	TRP	-	insertion	UNP Q93RN7
B	817	ILE	-	insertion	UNP Q93RN7
B	818	ASN	-	insertion	UNP Q93RN7
B	820	LEU	TRP	conflict	UNP Q93RN7
B	821	GLY	GLU	conflict	UNP Q93RN7
B	822	ASN	ILE	conflict	UNP Q93RN7
B	824	GLY	ALA	conflict	UNP Q93RN7
B	825	SER	LEU	conflict	UNP Q93RN7
B	826	ASP	THR	conflict	UNP Q93RN7
B	827	THR	ARG	conflict	UNP Q93RN7
B	828	LEU	TRP	conflict	UNP Q93RN7
B	829	ASP	ILE	conflict	UNP Q93RN7
B	830	MET	CYS	conflict	UNP Q93RN7
B	831	LEU	CYS	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	832	ARG	ALA	conflict	UNP Q93RN7
B	833	GLN	LYS	conflict	UNP Q93RN7
B	838	ALA	GLY	conflict	UNP Q93RN7
B	842	ALA	GLY	conflict	UNP Q93RN7
B	843	SER	LEU	conflict	UNP Q93RN7
B	844	VAL	ARG	conflict	UNP Q93RN7
B	845	MET	ASP	conflict	UNP Q93RN7
B	847	LEU	ALA	conflict	UNP Q93RN7
B	848	ASP	GLY	conflict	UNP Q93RN7
B	849	ILE	HIS	conflict	UNP Q93RN7
B	850	SER	GLN	conflict	UNP Q93RN7
B	851	MET	TYR	conflict	UNP Q93RN7
B	852	VAL	GLY	conflict	UNP Q93RN7
B	853	THR	ASN	conflict	UNP Q93RN7
B	854	GLN	ALA	conflict	UNP Q93RN7
B	855	ALA	GLY	conflict	UNP Q93RN7
B	856	MET	HIS	conflict	UNP Q93RN7
B	857	VAL	GLY	conflict	UNP Q93RN7
B	872	THR	PRO	conflict	UNP Q93RN7
B	878	ASP	HIS	conflict	UNP Q93RN7
B	884	HIS	ILE	conflict	UNP Q93RN7
B	911	SER	ALA	conflict	UNP Q93RN7
B	914	GLU	LYS	conflict	UNP Q93RN7
B	923	GLU	ALA	conflict	UNP Q93RN7
B	1067	LYS	GLN	conflict	UNP Q93RN7
B	1075	ASP	GLU	conflict	UNP Q93RN7
B	1126	ASP	ASN	conflict	UNP Q93RN7
B	1250	LYS	VAL	conflict	UNP Q93RN7
B	1253	SER	PRO	conflict	UNP Q93RN7
B	1257	GLY	ASP	conflict	UNP Q93RN7
B	1258	SER	ASN	conflict	UNP Q93RN7
B	1514	ILE	VAL	conflict	UNP Q93RN7
B	1519	MET	VAL	conflict	UNP Q93RN7
B	1877	ASN	TYR	conflict	UNP Q93RN7
B	1880	MET	THR	conflict	UNP Q93RN7
B	1884	ILE	VAL	conflict	UNP Q93RN7
B	1920	THR	ALA	conflict	UNP Q93RN7
B	1943	GLY	VAL	conflict	UNP Q93RN7
B	1947	GLN	HIS	conflict	UNP Q93RN7
B	1959	MET	ALA	conflict	UNP Q93RN7
B	1961	GLY	ASP	conflict	UNP Q93RN7
B	1962	ARG	ASN	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1964	GLY	GLU	conflict	UNP Q93RN7
B	1966	SER	ALA	conflict	UNP Q93RN7
B	1967	LYS	THR	conflict	UNP Q93RN7
B	1968	ASN	GLN	conflict	UNP Q93RN7
B	1969	LEU	PRO	conflict	UNP Q93RN7
B	2028	THR	PRO	conflict	UNP Q93RN7
B	2057	THR	ALA	conflict	UNP Q93RN7
B	2149	LEU	PHE	conflict	UNP Q93RN7
B	2161	VAL	ALA	conflict	UNP Q93RN7
B	2164	ILE	VAL	conflict	UNP Q93RN7
B	2178	LEU	PHE	conflict	UNP Q93RN7
B	2430	LEU	PHE	conflict	UNP Q93RN7
C	172	HIS	PRO	conflict	UNP Q93RN7
C	343	ASN	HIS	conflict	UNP Q93RN7
C	344	ILE	VAL	conflict	UNP Q93RN7
C	360	ARG	CYS	conflict	UNP Q93RN7
C	365	VAL	ILE	conflict	UNP Q93RN7
C	377	ALA	SER	conflict	UNP Q93RN7
C	379	PRO	THR	conflict	UNP Q93RN7
C	391	ILE	VAL	conflict	UNP Q93RN7
C	407	SER	ASN	conflict	UNP Q93RN7
C	410	LYS	ARG	conflict	UNP Q93RN7
C	566	VAL	ILE	conflict	UNP Q93RN7
C	583	ALA	THR	conflict	UNP Q93RN7
C	586	THR	ILE	conflict	UNP Q93RN7
C	587	ILE	LEU	conflict	UNP Q93RN7
C	592	PHE	PRO	conflict	UNP Q93RN7
C	606	VAL	ALA	conflict	UNP Q93RN7
C	620	LEU	PHE	conflict	UNP Q93RN7
C	637	PRO	SER	conflict	UNP Q93RN7
C	682	ASN	THR	conflict	UNP Q93RN7
C	686	SER	ARG	conflict	UNP Q93RN7
C	695	HIS	SER	conflict	UNP Q93RN7
C	696	ASN	ASP	conflict	UNP Q93RN7
C	736	ASP	ASN	conflict	UNP Q93RN7
C	742	THR	MET	conflict	UNP Q93RN7
C	748	SER	THR	conflict	UNP Q93RN7
C	750	ASN	SER	conflict	UNP Q93RN7
C	751	ALA	ASP	conflict	UNP Q93RN7
C	752	ASN	GLU	conflict	UNP Q93RN7
C	788	GLY	ASP	conflict	UNP Q93RN7
C	790	ALA	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	795	LYS	ARG	conflict	UNP Q93RN7
C	796	ASN	SER	conflict	UNP Q93RN7
C	799	ALA	PRO	conflict	UNP Q93RN7
C	800	GLY	ASP	conflict	UNP Q93RN7
C	801	GLN	ASN	conflict	UNP Q93RN7
C	?	-	THR	deletion	UNP Q93RN7
C	?	-	ILE	deletion	UNP Q93RN7
C	?	-	LEU	deletion	UNP Q93RN7
C	?	-	ILE	deletion	UNP Q93RN7
C	?	-	LEU	deletion	UNP Q93RN7
C	?	-	CYS	deletion	UNP Q93RN7
C	?	-	SER	deletion	UNP Q93RN7
C	803	ASN	SER	conflict	UNP Q93RN7
C	804	ILE	THR	conflict	UNP Q93RN7
C	806	THR	SER	conflict	UNP Q93RN7
C	807	LEU	THR	conflict	UNP Q93RN7
C	808	PHE	SER	conflict	UNP Q93RN7
C	809	SER	GLY	conflict	UNP Q93RN7
C	811	TYR	MET	conflict	UNP Q93RN7
C	812	ARG	-	insertion	UNP Q93RN7
C	813	PHE	-	insertion	UNP Q93RN7
C	814	HIS	-	insertion	UNP Q93RN7
C	815	GLN	-	insertion	UNP Q93RN7
C	816	TRP	-	insertion	UNP Q93RN7
C	817	ILE	-	insertion	UNP Q93RN7
C	818	ASN	-	insertion	UNP Q93RN7
C	820	LEU	TRP	conflict	UNP Q93RN7
C	821	GLY	GLU	conflict	UNP Q93RN7
C	822	ASN	ILE	conflict	UNP Q93RN7
C	824	GLY	ALA	conflict	UNP Q93RN7
C	825	SER	LEU	conflict	UNP Q93RN7
C	826	ASP	THR	conflict	UNP Q93RN7
C	827	THR	ARG	conflict	UNP Q93RN7
C	828	LEU	TRP	conflict	UNP Q93RN7
C	829	ASP	ILE	conflict	UNP Q93RN7
C	830	MET	CYS	conflict	UNP Q93RN7
C	831	LEU	CYS	conflict	UNP Q93RN7
C	832	ARG	ALA	conflict	UNP Q93RN7
C	833	GLN	LYS	conflict	UNP Q93RN7
C	838	ALA	GLY	conflict	UNP Q93RN7
C	842	ALA	GLY	conflict	UNP Q93RN7
C	843	SER	LEU	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	844	VAL	ARG	conflict	UNP Q93RN7
C	845	MET	ASP	conflict	UNP Q93RN7
C	847	LEU	ALA	conflict	UNP Q93RN7
C	848	ASP	GLY	conflict	UNP Q93RN7
C	849	ILE	HIS	conflict	UNP Q93RN7
C	850	SER	GLN	conflict	UNP Q93RN7
C	851	MET	TYR	conflict	UNP Q93RN7
C	852	VAL	GLY	conflict	UNP Q93RN7
C	853	THR	ASN	conflict	UNP Q93RN7
C	854	GLN	ALA	conflict	UNP Q93RN7
C	855	ALA	GLY	conflict	UNP Q93RN7
C	856	MET	HIS	conflict	UNP Q93RN7
C	857	VAL	GLY	conflict	UNP Q93RN7
C	872	THR	PRO	conflict	UNP Q93RN7
C	878	ASP	HIS	conflict	UNP Q93RN7
C	884	HIS	ILE	conflict	UNP Q93RN7
C	911	SER	ALA	conflict	UNP Q93RN7
C	914	GLU	LYS	conflict	UNP Q93RN7
C	923	GLU	ALA	conflict	UNP Q93RN7
C	1067	LYS	GLN	conflict	UNP Q93RN7
C	1075	ASP	GLU	conflict	UNP Q93RN7
C	1126	ASP	ASN	conflict	UNP Q93RN7
C	1250	LYS	VAL	conflict	UNP Q93RN7
C	1253	SER	PRO	conflict	UNP Q93RN7
C	1257	GLY	ASP	conflict	UNP Q93RN7
C	1258	SER	ASN	conflict	UNP Q93RN7
C	1514	ILE	VAL	conflict	UNP Q93RN7
C	1519	MET	VAL	conflict	UNP Q93RN7
C	1877	ASN	TYR	conflict	UNP Q93RN7
C	1880	MET	THR	conflict	UNP Q93RN7
C	1884	ILE	VAL	conflict	UNP Q93RN7
C	1920	THR	ALA	conflict	UNP Q93RN7
C	1943	GLY	VAL	conflict	UNP Q93RN7
C	1947	GLN	HIS	conflict	UNP Q93RN7
C	1959	MET	ALA	conflict	UNP Q93RN7
C	1961	GLY	ASP	conflict	UNP Q93RN7
C	1962	ARG	ASN	conflict	UNP Q93RN7
C	1964	GLY	GLU	conflict	UNP Q93RN7
C	1966	SER	ALA	conflict	UNP Q93RN7
C	1967	LYS	THR	conflict	UNP Q93RN7
C	1968	ASN	GLN	conflict	UNP Q93RN7
C	1969	LEU	PRO	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2028	THR	PRO	conflict	UNP Q93RN7
C	2057	THR	ALA	conflict	UNP Q93RN7
C	2149	LEU	PHE	conflict	UNP Q93RN7
C	2161	VAL	ALA	conflict	UNP Q93RN7
C	2164	ILE	VAL	conflict	UNP Q93RN7
C	2178	LEU	PHE	conflict	UNP Q93RN7
C	2430	LEU	PHE	conflict	UNP Q93RN7
D	172	HIS	PRO	conflict	UNP Q93RN7
D	343	ASN	HIS	conflict	UNP Q93RN7
D	344	ILE	VAL	conflict	UNP Q93RN7
D	360	ARG	CYS	conflict	UNP Q93RN7
D	365	VAL	ILE	conflict	UNP Q93RN7
D	377	ALA	SER	conflict	UNP Q93RN7
D	379	PRO	THR	conflict	UNP Q93RN7
D	391	ILE	VAL	conflict	UNP Q93RN7
D	407	SER	ASN	conflict	UNP Q93RN7
D	410	LYS	ARG	conflict	UNP Q93RN7
D	566	VAL	ILE	conflict	UNP Q93RN7
D	583	ALA	THR	conflict	UNP Q93RN7
D	586	THR	ILE	conflict	UNP Q93RN7
D	587	ILE	LEU	conflict	UNP Q93RN7
D	592	PHE	PRO	conflict	UNP Q93RN7
D	606	VAL	ALA	conflict	UNP Q93RN7
D	620	LEU	PHE	conflict	UNP Q93RN7
D	637	PRO	SER	conflict	UNP Q93RN7
D	682	ASN	THR	conflict	UNP Q93RN7
D	686	SER	ARG	conflict	UNP Q93RN7
D	695	HIS	SER	conflict	UNP Q93RN7
D	696	ASN	ASP	conflict	UNP Q93RN7
D	736	ASP	ASN	conflict	UNP Q93RN7
D	742	THR	MET	conflict	UNP Q93RN7
D	748	SER	THR	conflict	UNP Q93RN7
D	750	ASN	SER	conflict	UNP Q93RN7
D	751	ALA	ASP	conflict	UNP Q93RN7
D	752	ASN	GLU	conflict	UNP Q93RN7
D	788	GLY	ASP	conflict	UNP Q93RN7
D	790	ALA	VAL	conflict	UNP Q93RN7
D	795	LYS	ARG	conflict	UNP Q93RN7
D	796	ASN	SER	conflict	UNP Q93RN7
D	799	ALA	PRO	conflict	UNP Q93RN7
D	800	GLY	ASP	conflict	UNP Q93RN7
D	801	GLN	ASN	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	THR	deletion	UNP Q93RN7
D	?	-	ILE	deletion	UNP Q93RN7
D	?	-	LEU	deletion	UNP Q93RN7
D	?	-	ILE	deletion	UNP Q93RN7
D	?	-	LEU	deletion	UNP Q93RN7
D	?	-	CYS	deletion	UNP Q93RN7
D	?	-	SER	deletion	UNP Q93RN7
D	803	ASN	SER	conflict	UNP Q93RN7
D	804	ILE	THR	conflict	UNP Q93RN7
D	806	THR	SER	conflict	UNP Q93RN7
D	807	LEU	THR	conflict	UNP Q93RN7
D	808	PHE	SER	conflict	UNP Q93RN7
D	809	SER	GLY	conflict	UNP Q93RN7
D	811	TYR	MET	conflict	UNP Q93RN7
D	812	ARG	-	insertion	UNP Q93RN7
D	813	PHE	-	insertion	UNP Q93RN7
D	814	HIS	-	insertion	UNP Q93RN7
D	815	GLN	-	insertion	UNP Q93RN7
D	816	TRP	-	insertion	UNP Q93RN7
D	817	ILE	-	insertion	UNP Q93RN7
D	818	ASN	-	insertion	UNP Q93RN7
D	820	LEU	TRP	conflict	UNP Q93RN7
D	821	GLY	GLU	conflict	UNP Q93RN7
D	822	ASN	ILE	conflict	UNP Q93RN7
D	824	GLY	ALA	conflict	UNP Q93RN7
D	825	SER	LEU	conflict	UNP Q93RN7
D	826	ASP	THR	conflict	UNP Q93RN7
D	827	THR	ARG	conflict	UNP Q93RN7
D	828	LEU	TRP	conflict	UNP Q93RN7
D	829	ASP	ILE	conflict	UNP Q93RN7
D	830	MET	CYS	conflict	UNP Q93RN7
D	831	LEU	CYS	conflict	UNP Q93RN7
D	832	ARG	ALA	conflict	UNP Q93RN7
D	833	GLN	LYS	conflict	UNP Q93RN7
D	838	ALA	GLY	conflict	UNP Q93RN7
D	842	ALA	GLY	conflict	UNP Q93RN7
D	843	SER	LEU	conflict	UNP Q93RN7
D	844	VAL	ARG	conflict	UNP Q93RN7
D	845	MET	ASP	conflict	UNP Q93RN7
D	847	LEU	ALA	conflict	UNP Q93RN7
D	848	ASP	GLY	conflict	UNP Q93RN7
D	849	ILE	HIS	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	850	SER	GLN	conflict	UNP Q93RN7
D	851	MET	TYR	conflict	UNP Q93RN7
D	852	VAL	GLY	conflict	UNP Q93RN7
D	853	THR	ASN	conflict	UNP Q93RN7
D	854	GLN	ALA	conflict	UNP Q93RN7
D	855	ALA	GLY	conflict	UNP Q93RN7
D	856	MET	HIS	conflict	UNP Q93RN7
D	857	VAL	GLY	conflict	UNP Q93RN7
D	872	THR	PRO	conflict	UNP Q93RN7
D	878	ASP	HIS	conflict	UNP Q93RN7
D	884	HIS	ILE	conflict	UNP Q93RN7
D	911	SER	ALA	conflict	UNP Q93RN7
D	914	GLU	LYS	conflict	UNP Q93RN7
D	923	GLU	ALA	conflict	UNP Q93RN7
D	1067	LYS	GLN	conflict	UNP Q93RN7
D	1075	ASP	GLU	conflict	UNP Q93RN7
D	1126	ASP	ASN	conflict	UNP Q93RN7
D	1250	LYS	VAL	conflict	UNP Q93RN7
D	1253	SER	PRO	conflict	UNP Q93RN7
D	1257	GLY	ASP	conflict	UNP Q93RN7
D	1258	SER	ASN	conflict	UNP Q93RN7
D	1514	ILE	VAL	conflict	UNP Q93RN7
D	1519	MET	VAL	conflict	UNP Q93RN7
D	1877	ASN	TYR	conflict	UNP Q93RN7
D	1880	MET	THR	conflict	UNP Q93RN7
D	1884	ILE	VAL	conflict	UNP Q93RN7
D	1920	THR	ALA	conflict	UNP Q93RN7
D	1943	GLY	VAL	conflict	UNP Q93RN7
D	1947	GLN	HIS	conflict	UNP Q93RN7
D	1959	MET	ALA	conflict	UNP Q93RN7
D	1961	GLY	ASP	conflict	UNP Q93RN7
D	1962	ARG	ASN	conflict	UNP Q93RN7
D	1964	GLY	GLU	conflict	UNP Q93RN7
D	1966	SER	ALA	conflict	UNP Q93RN7
D	1967	LYS	THR	conflict	UNP Q93RN7
D	1968	ASN	GLN	conflict	UNP Q93RN7
D	1969	LEU	PRO	conflict	UNP Q93RN7
D	2028	THR	PRO	conflict	UNP Q93RN7
D	2057	THR	ALA	conflict	UNP Q93RN7
D	2149	LEU	PHE	conflict	UNP Q93RN7
D	2161	VAL	ALA	conflict	UNP Q93RN7
D	2164	ILE	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2178	LEU	PHE	conflict	UNP Q93RN7
D	2430	LEU	PHE	conflict	UNP Q93RN7
E	172	HIS	PRO	conflict	UNP Q93RN7
E	343	ASN	HIS	conflict	UNP Q93RN7
E	344	ILE	VAL	conflict	UNP Q93RN7
E	360	ARG	CYS	conflict	UNP Q93RN7
E	365	VAL	ILE	conflict	UNP Q93RN7
E	377	ALA	SER	conflict	UNP Q93RN7
E	379	PRO	THR	conflict	UNP Q93RN7
E	391	ILE	VAL	conflict	UNP Q93RN7
E	407	SER	ASN	conflict	UNP Q93RN7
E	410	LYS	ARG	conflict	UNP Q93RN7
E	566	VAL	ILE	conflict	UNP Q93RN7
E	583	ALA	THR	conflict	UNP Q93RN7
E	586	THR	ILE	conflict	UNP Q93RN7
E	587	ILE	LEU	conflict	UNP Q93RN7
E	592	PHE	PRO	conflict	UNP Q93RN7
E	606	VAL	ALA	conflict	UNP Q93RN7
E	620	LEU	PHE	conflict	UNP Q93RN7
E	637	PRO	SER	conflict	UNP Q93RN7
E	682	ASN	THR	conflict	UNP Q93RN7
E	686	SER	ARG	conflict	UNP Q93RN7
E	695	HIS	SER	conflict	UNP Q93RN7
E	696	ASN	ASP	conflict	UNP Q93RN7
E	736	ASP	ASN	conflict	UNP Q93RN7
E	742	THR	MET	conflict	UNP Q93RN7
E	748	SER	THR	conflict	UNP Q93RN7
E	750	ASN	SER	conflict	UNP Q93RN7
E	751	ALA	ASP	conflict	UNP Q93RN7
E	752	ASN	GLU	conflict	UNP Q93RN7
E	788	GLY	ASP	conflict	UNP Q93RN7
E	790	ALA	VAL	conflict	UNP Q93RN7
E	795	LYS	ARG	conflict	UNP Q93RN7
E	796	ASN	SER	conflict	UNP Q93RN7
E	799	ALA	PRO	conflict	UNP Q93RN7
E	800	GLY	ASP	conflict	UNP Q93RN7
E	801	GLN	ASN	conflict	UNP Q93RN7
E	?	-	THR	deletion	UNP Q93RN7
E	?	-	ILE	deletion	UNP Q93RN7
E	?	-	LEU	deletion	UNP Q93RN7
E	?	-	ILE	deletion	UNP Q93RN7
E	?	-	LEU	deletion	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	CYS	deletion	UNP Q93RN7
E	?	-	SER	deletion	UNP Q93RN7
E	803	ASN	SER	conflict	UNP Q93RN7
E	804	ILE	THR	conflict	UNP Q93RN7
E	806	THR	SER	conflict	UNP Q93RN7
E	807	LEU	THR	conflict	UNP Q93RN7
E	808	PHE	SER	conflict	UNP Q93RN7
E	809	SER	GLY	conflict	UNP Q93RN7
E	811	TYR	MET	conflict	UNP Q93RN7
E	812	ARG	-	insertion	UNP Q93RN7
E	813	PHE	-	insertion	UNP Q93RN7
E	814	HIS	-	insertion	UNP Q93RN7
E	815	GLN	-	insertion	UNP Q93RN7
E	816	TRP	-	insertion	UNP Q93RN7
E	817	ILE	-	insertion	UNP Q93RN7
E	818	ASN	-	insertion	UNP Q93RN7
E	820	LEU	TRP	conflict	UNP Q93RN7
E	821	GLY	GLU	conflict	UNP Q93RN7
E	822	ASN	ILE	conflict	UNP Q93RN7
E	824	GLY	ALA	conflict	UNP Q93RN7
E	825	SER	LEU	conflict	UNP Q93RN7
E	826	ASP	THR	conflict	UNP Q93RN7
E	827	THR	ARG	conflict	UNP Q93RN7
E	828	LEU	TRP	conflict	UNP Q93RN7
E	829	ASP	ILE	conflict	UNP Q93RN7
E	830	MET	CYS	conflict	UNP Q93RN7
E	831	LEU	CYS	conflict	UNP Q93RN7
E	832	ARG	ALA	conflict	UNP Q93RN7
E	833	GLN	LYS	conflict	UNP Q93RN7
E	838	ALA	GLY	conflict	UNP Q93RN7
E	842	ALA	GLY	conflict	UNP Q93RN7
E	843	SER	LEU	conflict	UNP Q93RN7
E	844	VAL	ARG	conflict	UNP Q93RN7
E	845	MET	ASP	conflict	UNP Q93RN7
E	847	LEU	ALA	conflict	UNP Q93RN7
E	848	ASP	GLY	conflict	UNP Q93RN7
E	849	ILE	HIS	conflict	UNP Q93RN7
E	850	SER	GLN	conflict	UNP Q93RN7
E	851	MET	TYR	conflict	UNP Q93RN7
E	852	VAL	GLY	conflict	UNP Q93RN7
E	853	THR	ASN	conflict	UNP Q93RN7
E	854	GLN	ALA	conflict	UNP Q93RN7

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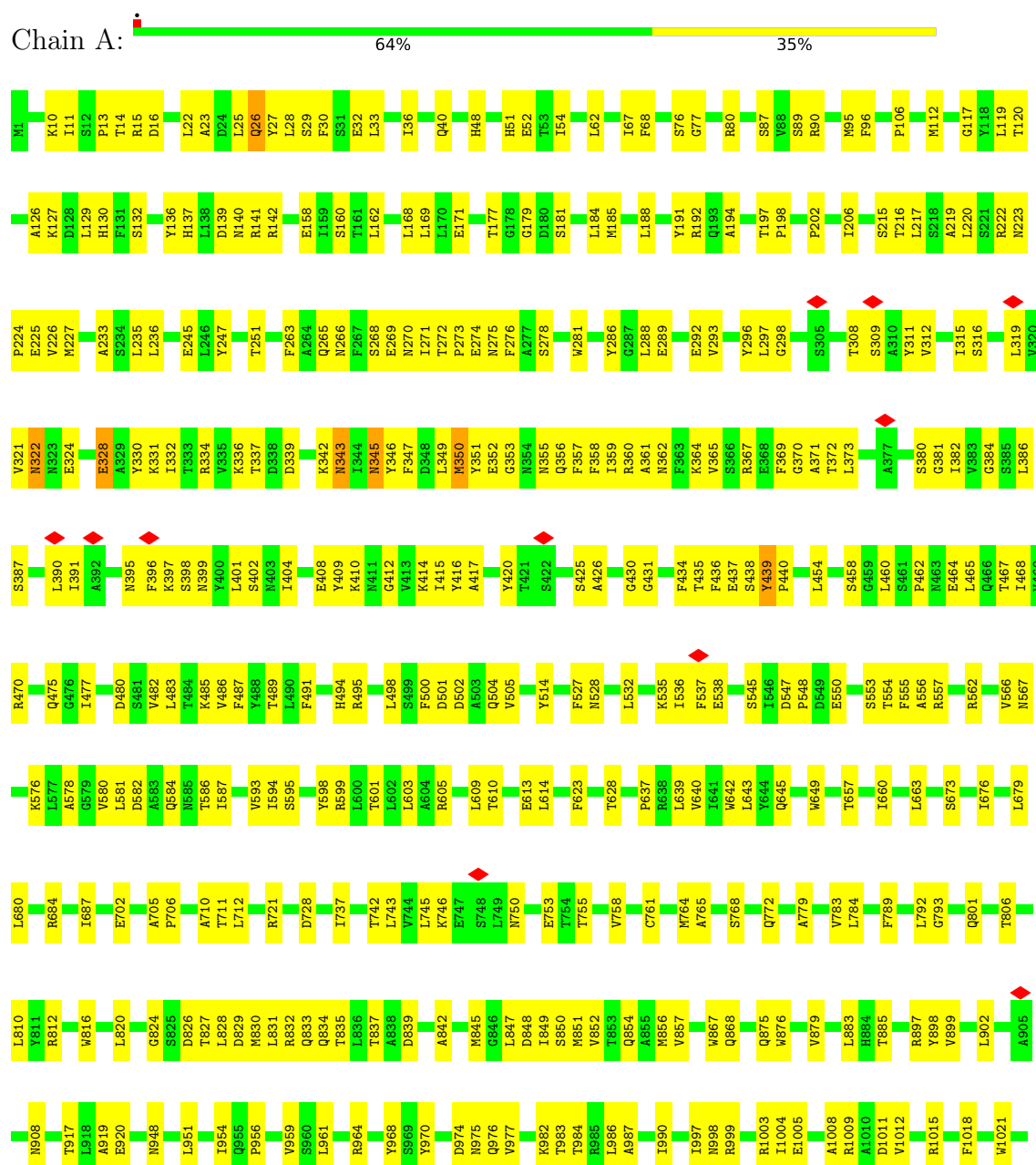
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Chain	Residue	Modelled	Actual	Comment	Reference
E	855	ALA	GLY	conflict	UNP Q93RN7
E	856	MET	HIS	conflict	UNP Q93RN7
E	857	VAL	GLY	conflict	UNP Q93RN7
E	872	THR	PRO	conflict	UNP Q93RN7
E	878	ASP	HIS	conflict	UNP Q93RN7
E	884	HIS	ILE	conflict	UNP Q93RN7
E	911	SER	ALA	conflict	UNP Q93RN7
E	914	GLU	LYS	conflict	UNP Q93RN7
E	923	GLU	ALA	conflict	UNP Q93RN7
E	1067	LYS	GLN	conflict	UNP Q93RN7
E	1075	ASP	GLU	conflict	UNP Q93RN7
E	1126	ASP	ASN	conflict	UNP Q93RN7
E	1250	LYS	VAL	conflict	UNP Q93RN7
E	1253	SER	PRO	conflict	UNP Q93RN7
E	1257	GLY	ASP	conflict	UNP Q93RN7
E	1258	SER	ASN	conflict	UNP Q93RN7
E	1514	ILE	VAL	conflict	UNP Q93RN7
E	1519	MET	VAL	conflict	UNP Q93RN7
E	1877	ASN	TYR	conflict	UNP Q93RN7
E	1880	MET	THR	conflict	UNP Q93RN7
E	1884	ILE	VAL	conflict	UNP Q93RN7
E	1920	THR	ALA	conflict	UNP Q93RN7
E	1943	GLY	VAL	conflict	UNP Q93RN7
E	1947	GLN	HIS	conflict	UNP Q93RN7
E	1959	MET	ALA	conflict	UNP Q93RN7
E	1961	GLY	ASP	conflict	UNP Q93RN7
E	1962	ARG	ASN	conflict	UNP Q93RN7
E	1964	GLY	GLU	conflict	UNP Q93RN7
E	1966	SER	ALA	conflict	UNP Q93RN7
E	1967	LYS	THR	conflict	UNP Q93RN7
E	1968	ASN	GLN	conflict	UNP Q93RN7
E	1969	LEU	PRO	conflict	UNP Q93RN7
E	2028	THR	PRO	conflict	UNP Q93RN7
E	2057	THR	ALA	conflict	UNP Q93RN7
E	2149	LEU	PHE	conflict	UNP Q93RN7
E	2161	VAL	ALA	conflict	UNP Q93RN7
E	2164	ILE	VAL	conflict	UNP Q93RN7
E	2178	LEU	PHE	conflict	UNP Q93RN7
E	2430	LEU	PHE	conflict	UNP Q93RN7

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: XptA2 protein



F2484	V2366	Q2262	V2161	Q2063	L1969	P1847	G1726	R1604	I1514	H1428	I1338	K1221	W1122	R1025
L2368	S2367	A2263	L2162	Q2066	R1970	W1848	V1727	Y1618	K1515	L1429	I1339	K1222	R1123	R1026
A2369	L2369	H2264	S2163	Q2066	L1975	N1851	G1728	Y1729	T1517	M1430	Q1340	E1226	N1124	T1029
Q2370	Q2370	Q2266	T2164	T2069	V1976	K1852	Q1730	L1626	V1518	R1436	I1341	D1126	V1125	
F2371	F2372	A2267	A2165	T2069	F1979	R1853	K1731	Q1629	M1519	R1437	T1342	A1229	L1127	
P2495	V2372	Q2268	N2174	M2074	L1980	P1854	I1732	Q1629	M1519	L1438	L1230	A1230	Y1038	
L2375	L2269	E2270	L2178	D2079	P1981	L1855	T1733	R1633	K1523	L1439	A1351	A1231	M1130	
L2382	L2271	L2272	L2184	L2088	Y1983	P1865	F1742	R1633	F1527	L1440	I1352	Q1236	A1132	E1041
F2389	R2184	K2275	W2185	L2088	M1984	D1870	Y1743	T1638	S1530	P1442	L1354	T1240	P1046	
L2390	W2185	K2278	G2186	A2095	L1987	P1871	F1745	T1640	D1531	R1450	H1355	L1241	W1140	P1046
R2391	G2186	N2278	K2279	T2096	L1987	D1872	E1746	L1641	H1532	L1451	I1352	Q1236	I1047	
E2392	L2189	K2279	R2190	Q2097	W1991	A1874	T1748	T1643	I1533	F1452	A1358	F1244	W1143	Q1048
Q2393	L2190	K2279	A2191	S2098	Q1992	A1875	T1748	T1643	S1535	F1454	D1364	Y1245	T1148	I0501
K2394	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
G2395	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
S2400	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
K2405	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2406	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
V2415	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
R2416	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2417	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2420	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
K2421	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2422	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
R2434	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
Q2435	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2436	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
K2437	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
Q2438	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
V2439	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
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V2456	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2457	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
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Y2459	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
G2460	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
G2461	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
C2469	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
L2472	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
K2473	L2190	T2099	A2191	S2098	T1993	H1881	I1755	E1645	L1536	F1455	G1365	K1247	A1149	Q1052
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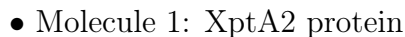


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	P2449	L2341	L2241	E2142	P2051	D1926	A1826	Y1718	L1601	Q1499	Y1421	
	Y2450	L2342	E2242	E2146	M2052	E1927	T1827	M1719	F1602	G1508	A1423	P1316
	E2451	L2343	K2245	M2146	M2053	E1927	Q1828	H1720	L1603	S1318	S1424	S1317
	R2454	N2344	L2246	L2157	L2054	L1960	W1828	E1721	R1604	N1510	L1319	L1319
	A2455	L2345	K2247	L2157	E2055	L1960	I1830	G1722	A1610	N1511	W1320	W1320
	V2456	A2346	R2248	L2157	R2056	G1963	M1831	G1722	Q1611	T1514	M1321	M1321
	L2457	E2249	R2248	S2163	T2057	G1964	Y1832	L1725	Y1434	K1515	T1331	T1331
	N2458	M2348	A2250	T2164	R2058	V1965	Y1833	G1726	T1435	T1516	V1332	V1332
	Y2459	A2251	A2250	A2165	N2059	S1966	Y1834	V1727	R1436	T1517	R1436	R1436
	G2460	K2350	Q2252	E2166	L2060	K1967	Y1834	G1728	R1437	V1518	R1437	Q1340
	G2461	M2253	M2253	E2166	V2061	N1968	G1838	Y1729	L1438	M1519	T1341	T1341
	M2465	Q2254	Q2254	N2174	A2062	L1969	Y1839	Q1730	L1440	K1523	T1441	T1441
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	T2472	Q2261	Q2261	G2182	Q2066	V1976	W1848	F1742	S1628	S1530	A1351	A1351
	A2473	H2264	H2264	R2183	L2083	P1981	M1851	F1743	Q1629	D1531	T1352	T1352
	L2474	L2269	L2269	W2185	L2088	P1981	C1852	T1749	L1630	H1532	T1353	T1353
	G2477	L2269	L2269	G2186	Q2089	Y1990	R1853	Q1760	L1631	T1353	L1354	L1354
	F2484	R2274	R2274	A2187	Q2090	W1991	P1854	Q1751	S1632	A1534	H1355	H1355
	M2485	K2275	K2275	A2191	E2093	R1995	W1861	I1755	D1639	F1541	R1362	R1362
	Y2493	W2284	W2284	S2192	A2095	L1998	N1862	S1762	T1640	F1548	Y1363	Y1363
	L2494	M2285	M2285	V2195	L2099	F1989	D1872	G1763	I1641	E1552	N1368	N1368
	P2495	K2288	K2288	L2198	R2100	N2000	D1878	Q1766	L1642	T1553	V1369	V1369
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	S2510	C2304	C2304	K2209	D2110	S2013	M1888	Y1788	E1651	D1568	F1466	F1466
	P2511	L2305	L2305	Y2216	D2112	L2014	R1889	Y1788	P1652	I1569	T1467	T1467
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	D2513	A2307	A2307	E2222	A2114	L2016	L1891	M1792	F1659	F1571	T1473	T1473
	A2514	Q2308	Q2308	Q2221	V2115	Y2017	D1892	A1797	L1664	E1572	F1476	F1476
	T2515	L2311	L2311	E2224	L2116	A2018	Q1893	A1797	E1675	K1574	C1479	C1479
	D2516	R2312	R2312	Q2224	R2120	E2019	L1894	E1804	E1675	A1575	V1483	V1483
	K2519	Q2321	Q2321	Q2226	Q2124	P2020	R1897	Y1808	W1677	K1576	D1484	D1484
	D2527	F2322	F2322	N2229	N2125	T2021	G1898	T1809	F1678	L1581	G1485	G1485
		I2323	I2323	D2231	R2126	T2022	Y1902	P1810	K1679	T1584	N1486	N1486
					L2127	P2023	M1811	M1811	L1699	K1585	S1488	S1488
					E2128	L2026	L2027	M1812		Q1586	Q1489	Q1489
						T2028						

• Molecule 1: XptA2 protein



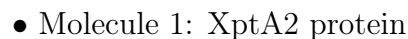




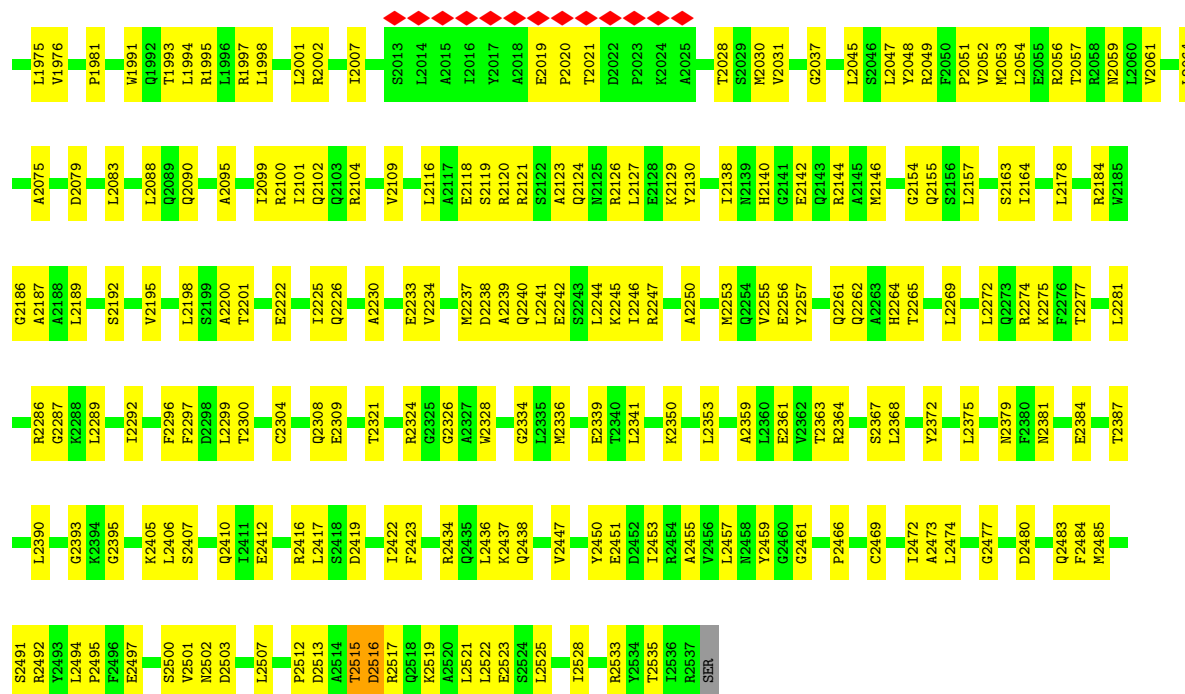
Response	Percentage
Democracy	64%
Dictatorship	36%



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S1540	Y1447	V1369	K1250	W1030	M922	S825	L712	S826	D502	G412	I332	T251
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F1548	E1453	Q1374	M1286	I1044	W949	D829	R721	L602	N507	I415	K342	K257
X1549	F1454	I1375	I1267	D1045	F950	N830	L725	L603	Y420	N345	A259	N258
P1550	F1456	A1377	M1276	P1046	N953	R831	D728	R605	T421	Y346	K343	Q265
L1551	S1457	M1378	M1277	R1049	N954	R832	P732	V606	S521	F347	N344	R266
A1555	P1458	K1379	M1280	I1050	Q955	R840	I737	H607	H522	F348	E269	F267
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D1568	F1466	R1163	K1288	S1067	L964	D848	L745	K746	L532	F436	E274	T273
I1569	T1467	R1165	N1289	K1067	R964	I849	L746	K746	K533	E437	N275	E274
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K1576	T1473	I1169	H1295	T1079	S969	V861	F760	Q645	S545	T442	Q279	Q279
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K1583	F1475	V1171	Y1081	Y1081	Y971	V861	M764	W649	I546	I444	A361	A361
I1584	F1476	E1174	K1304	T1082	L972	W867	S768	A653	D547	F444	N362	I282
K1585	K1477	E1175	S1305	R1083	T973	I870	L769	A653	P548	L446	S366	Y286
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V1593	Y1481	Y1187	F1309	T1086	Q976	W875	Q772	I660	Q552	R453	E291	E291
I1600	V1413	T1191	S1318	A1088	I981	Q875	R775	W661	S553	L454	V293	V293
L1601	V1414	L1192	L1319	D1089	K982	W876	L776	L662	T554	C455	Q294	Q294
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Y1618	Q1489	R1198	M1333	V1100	R985	V879	E780	T665	R562	P462	L308	T308
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I1641	I1516	D1011	L1354	M1130	D1011	A905	F813	Q700	V580	Y400	E324	E324
K1644	K1523	G1237	H1355	Q1131	V1012	E906	Q815	I703	L581	L486	S325	S325
M1644	L1440	T1240	F1359	G1133	R1015	S907	Q815	L704	D582	F487	S402	S402
F1527	F1527	L1441				N908	W816	A705		Y488	M403	M403



A1846	A1847	A1714	I1620	G1508	K1417	A1317	A1205	R1114	T983	W867	E778	R684	K576	Q475	A392
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M1851	M1852	Y1718	N1623	K1515	Y1421	L1319	W1207	N1116	A987	D869	E780	E689	V580	I477	N395
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R1889	T1886	F1743	D1639	D1542	R1437	I1341	F1235	M1130	R1015	P887	G800	L712	L600	Y496	D406
L1890	T1886	F1743	T1640	A1543	L1440	L1350	F1244	L1136	R1015	H802	L714	H713	A804	L498	S407
D1892	Q1893	I1755	L1644	F1548	P1442	A1351	V1243	W1140	F1018	N897	N803	L724	V606	S499	E408
L1896	R1897	A1758	R1648	E1552	Y1447	H1355	Y1246	A1139	F1018	Y898	T806	A720	D501	G412	G412
Y1902	Y1902	H1760	L1649	I1553	F1452	Y1363	K1247	W1143	W1021	Y898	L810	A720	D501	Y413	Y413
A1913	R1914	Q1767	P1650	D1554	F1453	R1362	K1248	W1146	N1024	Y898	F813	A720	D501	K414	K414
M1915	W1916	I1784	L1664	I1569	F1461	R1362	K1248	D1147	N1025	Y898	W816	A720	D501	I415	I415
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R1918	R1918	Y1801	Y1667	E1572	T1467	L1380	K1274	A1149	E1041	Y898	G819	A720	D501	A417	A417
T1920	T1920	Y1801	D1668	T1573	V1468	T1381	K1275	N1151	E1041	Y898	L820	A720	D501	Y420	Y420
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G1932	G1932	P1810	R1676	L1581	C1479	Y1389	M1276	E1174	L1060	Y898	R840	A720	D501	G432	G432
S1933	Q1934	M1811	F1677	G1582	A1482	G1390	M1276	E1175	T1079	Y898	L841	A720	D501	I433	I433
Q1935	Q1935	M1812	K1679	I1584	A1482	G1390	M1276	D1182	L1081	Y898	A842	A720	D501	F434	F434
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Q1955	D1956	K1821	R1691	S1589	Q1489	V1399	M1276	L1192	R1083	Y898	V758	A720	D501	F436	F436
D1957	L1957	W1829	M1698	V1593	F1491	K1400	M1276	L1193	F1084	Y898	Q759	A720	D501	E437	E437
L1960	L1960	N1831	L1699	L1601	F1492	H1401	M1276	L1194	F1085	Y898	T554	A720	D501	I451	I451
G1963	G1963	Y1832	S1703	F1602	F1494	G1409	M1276	L1197	T1086	Y898	F555	A720	D501	R453	R453
Y1965	Y1965	Y1833	E1704	E1605	F1494	G1410	M1276	L1197	D1089	Y898	M851	A720	D501	P462	P462
S1967	N1968	G1838	F1710	Q1611	Y1497	I1412	M1276	D1200	Y1096	Y898	T853	A720	D501	M463	M463
Y1967	Y1967	Y1839	Y1713	M1613	Q1498	T1413	M1276	G1201	Y1096	Y898	Q854	A720	D501	E464	E464
N1968	N1968	Y1839	Y1713	M1613	S1499	Y1414	M1276	W1203	Y1096	Y898	A855	A720	D501	Q466	Q466
					T1507	N1416	M1276	S1204	L1106	Y898	M856	A720	D501	T467	T467
											V861	A720	D501	I468	I468



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	42561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00379	Depositor
Map size (Å)	438.728, 438.728, 438.728	wwPDB
Map dimensions	346, 346, 346	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/20412	0.50	4/27712 (0.0%)
1	B	0.28	0/20413	0.52	5/27714 (0.0%)
1	C	0.27	0/20413	0.49	6/27714 (0.0%)
1	D	0.27	0/20413	0.51	5/27714 (0.0%)
1	E	0.28	0/20413	0.53	6/27714 (0.0%)
All	All	0.27	0/102064	0.51	26/138568 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	7
All	All	0	21

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2515	THR	CA-C-N	10.61	140.80	121.70
1	C	2515	THR	C-N-CA	10.61	140.80	121.70
1	D	2515	THR	CA-C-N	10.24	140.14	121.70
1	D	2515	THR	C-N-CA	10.24	140.14	121.70
1	B	2515	THR	CA-C-N	9.82	139.37	121.70
1	B	2515	THR	C-N-CA	9.82	139.37	121.70
1	E	2515	THR	CA-C-N	9.17	138.21	121.70
1	E	2515	THR	C-N-CA	9.17	138.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2515	THR	CA-C-N	8.62	137.21	121.70
1	A	2515	THR	C-N-CA	8.62	137.21	121.70
1	A	1056	MET	CB-CG-SD	-6.28	93.85	112.70
1	D	346	TYR	CA-CB-CG	6.26	125.18	113.90
1	D	359	ILE	CG1-CB-CG2	-6.25	91.96	110.70
1	E	2021	THR	CA-C-N	6.08	136.64	121.80
1	E	2021	THR	C-N-CA	6.08	136.64	121.80
1	D	322	ASN	N-CA-C	5.94	117.45	110.97
1	C	2021	THR	CA-C-N	5.91	136.23	121.80
1	C	2021	THR	C-N-CA	5.91	136.23	121.80
1	E	1387	SER	CB-CA-C	-5.77	109.39	117.23
1	E	323	ASN	N-CA-C	5.53	117.07	110.44
1	B	2128	GLU	N-CA-CB	5.50	118.76	110.30
1	B	1387	SER	CB-CA-C	-5.35	109.95	117.23
1	C	1387	SER	CB-CA-C	-5.30	110.03	117.23
1	A	1055	MET	CB-CG-SD	5.19	128.27	112.70
1	C	2516	ASP	N-CA-CB	5.19	119.32	110.50
1	B	2128	GLU	CA-CB-CG	5.10	124.30	114.10

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	GLN	Peptide
1	A	2515	THR	Peptide
1	A	26	GLN	Peptide
1	A	312	VAL	Peptide
1	A	322	ASN	Peptide
1	A	328	GLU	Peptide
1	A	345	ASN	Peptide
1	A	350	MET	Peptide
1	A	439	TYR	Peptide
1	B	362	ASN	Peptide
1	C	312	VAL	Peptide
1	D	26	GLN	Peptide
1	D	312	VAL	Peptide
1	D	345	ASN	Peptide
1	E	322	ASN	Peptide
1	E	328	GLU	Peptide
1	E	350	MET	Peptide
1	E	356	GLN	Peptide
1	E	362	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	439	TYR	Peptide
1	E	840	ARG	Sidechain

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	20006	0	19588	771	0
1	B	20007	0	19592	781	0
1	C	20007	0	19592	756	0
1	D	20007	0	19592	766	0
1	E	20007	0	19592	737	0
All	All	100034	0	97956	3637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (3637) 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:C:316:SER:HA	1:C:331:LYS:HE3	1.37	1.03
1:D:2515:THR:H	1:D:2516:ASP:HB2	1.19	1.03
1:E:369:PHE:HA	1:E:386:LEU:O	1.56	1.03
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.19	1.02
1:C:2242:GLU:HA	1:C:2245:LYS:HD3	1.43	0.99
1:A:1416:ASN:O	1:A:1420:ASN:HA	1.62	0.99
1:A:1053:THR:HB	1:A:1055:MET:HE2	1.46	0.98
1:E:1367:GLY:HA2	1:E:1371:ARG:HE	1.29	0.97
1:D:1367:GLY:HA2	1:D:1371:ARG:HE	1.30	0.96
1:A:369:PHE:HA	1:A:386:LEU:O	1.66	0.96
1:A:1440:LEU:HB2	1:A:1452:PHE:HB2	1.45	0.95
1:E:2120:ARG:HA	1:E:2237:MET:HE3	1.45	0.95
1:B:1117:LEU:HD21	1:C:1205:ALA:HB3	1.49	0.93
1:D:1437:ARG:HG2	1:D:1455:PRO:HA	1.48	0.93
1:E:2515:THR:H	1:E:2516:ASP:HB2	1.32	0.92
1:C:369:PHE:HA	1:C:386:LEU:O	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:PHE:HA	1:B:386:LEU:O	1.69	0.92
1:D:1439:ILE:HG23	1:D:1450:ARG:HG3	1.52	0.92
1:E:336:LYS:HG2	1:E:339:ASP:HB2	1.51	0.91
1:A:358:PHE:HB3	1:A:398:SER:HB3	1.53	0.91
1:D:1440:LEU:HB2	1:D:1452:PHE:HB2	1.50	0.90
1:C:28:LEU:HD12	1:C:32:GLU:HG2	1.52	0.90
1:C:1440:LEU:HB2	1:C:1452:PHE:HB2	1.50	0.90
1:B:350:MET:HE1	1:B:359:ILE:HA	1.53	0.90
1:A:964:ARG:HB3	1:A:976:GLN:HE22	1.36	0.89
1:C:1367:GLY:HA2	1:C:1371:ARG:HE	1.35	0.89
1:E:1440:LEU:HB2	1:E:1452:PHE:HB2	1.55	0.88
1:D:901:ALA:H	1:D:907:SER:HB2	1.39	0.88
1:C:2515:THR:H	1:C:2516:ASP:HB2	1.37	0.87
1:B:2026:LEU:HD21	1:C:818:ASN:HB3	1.57	0.86
1:B:2515:THR:N	1:B:2516:ASP:HB2	1.90	0.86
1:A:468:ILE:HD13	1:A:486:VAL:HG12	1.57	0.86
1:A:1647:GLN:HE22	1:A:1852:CYS:HA	1.40	0.86
1:C:901:ALA:H	1:C:907:SER:HB3	1.40	0.86
1:A:1117:LEU:HD21	1:B:1205:ALA:HB3	1.57	0.85
1:C:236:LEU:HD13	1:C:487:PHE:HB2	1.57	0.85
1:E:528:ASN:HD21	1:E:536:ILE:HB	1.42	0.85
1:E:1241:LEU:HB2	1:E:1267:ILE:HG22	1.58	0.85
1:E:1437:ARG:HG3	1:E:1455:PRO:HA	1.58	0.85
1:D:1649:LEU:HD12	1:D:1650:PRO:HD2	1.59	0.85
1:B:901:ALA:H	1:B:907:SER:HB2	1.43	0.84
1:C:360:ARG:HG2	1:C:365:VAL:HG22	1.60	0.84
1:B:708:ILE:O	1:B:712:LEU:HB3	1.77	0.84
1:C:358:PHE:HB3	1:C:398:SER:HB3	1.60	0.84
1:A:324:GLU:HB3	1:A:351:TYR:CE1	2.13	0.84
1:B:1416:ASN:O	1:B:1420:ASN:HA	1.78	0.83
1:B:1047:THR:HA	1:B:1812:MET:HE1	1.59	0.83
1:E:1416:ASN:O	1:E:1420:ASN:HA	1.79	0.83
1:B:2465:MET:HE1	1:B:2469:CYS:HB2	1.60	0.83
1:A:324:GLU:HB3	1:A:351:TYR:HE1	1.40	0.83
1:C:1340:GLN:HB3	1:C:1355:HIS:HB2	1.60	0.83
1:B:1487:ASN:H	1:B:1489:GLN:HE22	1.26	0.83
1:B:1399:VAL:HA	1:B:1498:GLN:O	1.79	0.82
1:A:2372:TYR:HA	1:A:2375:LEU:HD23	1.60	0.82
1:D:1422:ILE:HG12	1:D:1468:VAL:HG22	1.59	0.82
1:E:1722:GLY:H	1:E:1766:GLN:HG2	1.43	0.82
1:A:2372:TYR:HB2	1:A:2382:LEU:HD21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HD11	1:B:919:ALA:HA	1.61	0.82
1:B:649:TRP:HD1	1:B:812:ARG:HH12	1.26	0.82
1:A:528:ASN:HD21	1:A:536:ILE:HB	1.44	0.82
1:C:2465:MET:HG2	1:C:2466:PRO:HD2	1.62	0.82
1:E:95:MET:HE1	1:E:1968:ASN:HB3	1.62	0.81
1:E:330:TYR:HA	1:E:437:GLU:O	1.80	0.81
1:B:1362:ARG:HH21	1:B:1363:TYR:HB2	1.44	0.81
1:C:2037:GLY:HA3	1:C:2326:GLY:HA2	1.62	0.81
1:B:1742:PHE:HB3	1:B:1755:ILE:HD12	1.63	0.81
1:D:1241:LEU:HB2	1:D:1267:ILE:HG22	1.62	0.81
1:A:1742:PHE:HB3	1:A:1755:ILE:HD12	1.62	0.81
1:B:2494:LEU:HD12	1:B:2495:PRO:HD2	1.62	0.81
1:D:1742:PHE:HB3	1:D:1755:ILE:HD12	1.61	0.81
1:A:1399:VAL:HA	1:A:1498:GLN:O	1.82	0.80
1:D:1319:LEU:HD21	1:D:1586:GLN:HG2	1.63	0.80
1:E:1742:PHE:HB3	1:E:1755:ILE:HD12	1.61	0.80
1:D:1965:VAL:HG12	1:D:1967:LYS:H	1.45	0.80
1:B:1422:ILE:HG12	1:B:1468:VAL:HG22	1.64	0.80
1:D:249:ILE:HG22	1:D:450:LYS:HE3	1.61	0.80
1:B:318:GLY:HA2	1:B:329:ALA:HA	1.62	0.80
1:A:1241:LEU:HB2	1:A:1267:ILE:HG22	1.63	0.80
1:B:77:GLY:H	1:B:1925:GLY:HA3	1.43	0.80
1:D:28:LEU:HD12	1:D:32:GLU:HG2	1.63	0.80
1:B:1722:GLY:H	1:B:1766:GLN:HG2	1.47	0.80
1:E:1668:ASP:HB3	1:E:1671:GLU:HG2	1.62	0.80
1:C:528:ASN:HD21	1:C:536:ILE:HB	1.45	0.79
1:E:1422:ILE:HB	1:E:1466:PHE:HB2	1.63	0.79
1:B:198:PRO:HG3	1:B:245:GLU:HB3	1.64	0.79
1:B:1319:LEU:HD21	1:B:1586:GLN:HG2	1.65	0.79
1:C:1742:PHE:HB3	1:C:1755:ILE:HD12	1.64	0.79
1:A:95:MET:HE1	1:A:1968:ASN:HB3	1.65	0.79
1:A:1399:VAL:HG22	1:A:1499:SER:HA	1.65	0.79
1:A:761:CYS:HA	1:A:764:MET:HE2	1.63	0.78
1:D:77:GLY:H	1:D:1925:GLY:HA3	1.47	0.78
1:D:95:MET:HG2	1:D:1960:LEU:HD21	1.64	0.78
1:E:1115:GLU:HG3	1:E:1117:LEU:H	1.48	0.78
1:D:899:VAL:HG11	1:D:904:LYS:HB2	1.65	0.78
1:A:206:ILE:HD11	1:A:919:ALA:HA	1.65	0.78
1:A:2272:LEU:HD21	1:E:2083:LEU:HD12	1.65	0.78
1:B:1440:LEU:HB2	1:B:1452:PHE:HB2	1.64	0.78
1:D:2515:THR:N	1:D:2516:ASP:HB2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1439:ILE:HG23	1:E:1450:ARG:HG3	1.65	0.77
1:E:1053:THR:HG22	1:E:1055:MET:H	1.47	0.77
1:A:2051:PRO:HA	1:A:2054:LEU:HD12	1.64	0.77
1:A:346:TYR:HE1	1:A:360:ARG:HA	1.50	0.77
1:B:2142:GLU:HG2	1:B:2216:TYR:HE2	1.48	0.77
1:B:2465:MET:HG2	1:B:2466:PRO:HD2	1.65	0.77
1:C:826:ASP:O	1:C:829:ASP:HB3	1.85	0.77
1:C:2061:VAL:HA	1:C:2064:LEU:HD12	1.65	0.77
1:A:2148:LEU:HD22	1:B:2207:ALA:HB2	1.65	0.77
1:E:839:ASP:HA	1:E:849:ILE:HD13	1.66	0.76
1:D:2075:ALA:HA	1:D:2286:ARG:NH2	1.99	0.76
1:E:1965:VAL:HG12	1:E:1967:LYS:H	1.50	0.76
1:E:824:GLY:O	1:E:827:THR:HB	1.84	0.76
1:E:2457:LEU:HB2	1:E:2472:ILE:HG22	1.68	0.76
1:C:2455:ALA:HB3	1:C:2474:LEU:HB2	1.67	0.76
1:D:2130:TYR:HE1	1:E:2225:ILE:HD12	1.49	0.76
1:B:2250:ALA:HA	1:B:2253:MET:SD	2.26	0.76
1:E:1442:PRO:HD3	1:E:1451:LEU:HG	1.68	0.76
1:C:77:GLY:H	1:C:1925:GLY:HA3	1.49	0.76
1:B:1889:ARG:O	1:B:1892:ASP:HB2	1.86	0.75
1:B:26:GLN:HG3	1:B:27:TYR:HA	1.68	0.75
1:B:158:GLU:HG3	1:B:982:LYS:HG2	1.68	0.75
1:D:1890:LEU:O	1:D:1893:GLN:HG2	1.85	0.75
1:C:1333:MET:HE1	1:C:1582:GLY:HA3	1.66	0.75
1:A:2113:ILE:HG22	1:A:2244:LEU:HB3	1.69	0.75
1:E:2053:MET:HA	1:E:2056:ARG:HG2	1.67	0.75
1:D:760:PHE:HE1	1:D:764:MET:HE3	1.50	0.75
1:E:77:GLY:H	1:E:1925:GLY:HA3	1.52	0.75
1:B:820:LEU:HB3	1:B:824:GLY:HA3	1.68	0.75
1:E:1422:ILE:HG12	1:E:1468:VAL:HG22	1.69	0.75
1:A:824:GLY:O	1:A:827:THR:HB	1.87	0.74
1:A:554:THR:HG22	1:A:556:ALA:H	1.51	0.74
1:C:1117:LEU:HD13	1:E:2164:ILE:HG21	1.69	0.74
1:C:347:PHE:HB3	1:C:415:ILE:HG23	1.67	0.74
1:D:826:ASP:O	1:D:829:ASP:HB3	1.87	0.74
1:E:1574:LYS:HA	1:E:1581:LEU:H	1.52	0.74
1:A:1340:GLN:HB3	1:A:1355:HIS:HB2	1.67	0.74
1:A:2043:GLY:HA2	1:A:2305:LEU:HD13	1.69	0.74
1:D:1638:ILE:H	1:D:1638:ILE:HD12	1.53	0.74
1:C:2113:ILE:HG22	1:C:2244:LEU:HB3	1.70	0.74
1:D:2155:GLN:HE22	1:E:2200:ALA:HB2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:PHE:HB2	1:B:2485:MET:HE1	1.68	0.73
1:B:826:ASP:O	1:B:829:ASP:HB3	1.87	0.73
1:C:2515:THR:HB	1:C:2516:ASP:CG	2.12	0.73
1:E:349:LEU:HD13	1:E:356:GLN:HE21	1.52	0.73
1:E:1921:LEU:HD12	1:E:1994:LEU:HD21	1.68	0.73
1:D:2465:MET:HE1	1:D:2469:CYS:HB2	1.68	0.73
1:A:77:GLY:H	1:A:1925:GLY:HA3	1.52	0.73
1:D:1394:ILE:HG12	1:D:1417:LYS:HZ2	1.53	0.73
1:B:1117:LEU:HD12	1:D:2164:ILE:HG22	1.69	0.73
1:C:206:ILE:HD11	1:C:919:ALA:HA	1.69	0.73
1:D:1340:GLN:HB3	1:D:1355:HIS:HB2	1.70	0.73
1:E:348:ASP:H	1:E:359:ILE:HG22	1.53	0.73
1:A:28:LEU:HD12	1:A:32:GLU:HG2	1.70	0.73
1:A:1371:ARG:O	1:A:1375:ILE:HG12	1.88	0.73
1:A:1461:ILE:HG13	1:A:1463:ASN:H	1.52	0.73
1:C:820:LEU:HB3	1:C:824:GLY:HA3	1.71	0.73
1:D:1880:MET:O	1:D:1883:LYS:HB2	1.89	0.73
1:A:1422:ILE:HB	1:A:1466:PHE:HB2	1.71	0.73
1:E:2515:THR:N	1:E:2516:ASP:HB2	2.03	0.73
1:A:332:ILE:HD11	1:A:350:MET:HE3	1.71	0.72
1:B:1410:GLY:HA3	1:B:1497:TYR:HE2	1.54	0.72
1:C:1932:GLY:HA2	1:C:1935:GLN:HE21	1.54	0.72
1:A:2308:GLN:HE22	1:A:2321:THR:HG23	1.53	0.72
1:D:2250:ALA:HA	1:D:2253:MET:HE3	1.71	0.72
1:E:206:ILE:HD12	1:E:922:MET:HE3	1.70	0.72
1:A:1571:PHE:HB2	1:A:1584:ILE:HB	1.70	0.72
1:A:1764:MET:HE1	1:A:1769:ILE:HG13	1.71	0.72
1:C:1376:SER:HA	1:C:1379:LYS:HE3	1.72	0.72
1:E:406:ASP:HA	1:E:409:TYR:HB2	1.71	0.72
1:B:2031:VAL:HG12	1:C:779:ALA:HB3	1.72	0.72
1:E:2272:LEU:HD12	1:E:2275:LYS:HD2	1.72	0.72
1:C:505:VAL:HG11	1:C:598:TYR:HD2	1.55	0.72
1:C:1429:LEU:HD21	1:C:1436:ARG:HD3	1.71	0.72
1:B:256:GLU:HA	1:B:259:ALA:HB2	1.72	0.72
1:E:342:LYS:HD2	1:E:346:TYR:HB3	1.70	0.72
1:E:1333:MET:HE1	1:E:1582:GLY:HA3	1.71	0.72
1:B:105:LYS:HD3	1:B:106:PRO:HD2	1.72	0.71
1:A:1381:THR:HG21	1:A:1386:LYS:HA	1.71	0.71
1:C:2515:THR:N	1:C:2516:ASP:HB2	2.05	0.71
1:B:1442:PRO:HD3	1:B:1451:LEU:HG	1.72	0.71
1:C:1965:VAL:HG12	1:C:1967:LYS:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ARG:HG2	1:D:211:MET:HE1	1.71	0.71
1:D:2488:PHE:HB2	1:E:2485:MET:HE1	1.71	0.71
1:E:404:ILE:HG21	1:E:414:LYS:HD2	1.72	0.71
1:E:2045:LEU:HD13	1:E:2309:GLU:HG2	1.73	0.71
1:A:347:PHE:HD1	1:A:358:PHE:HZ	1.39	0.71
1:B:2061:VAL:HA	1:B:2064:LEU:HD12	1.71	0.71
1:C:1536:LEU:HD12	1:C:1537:PRO:HD2	1.72	0.71
1:E:1381:THR:HG21	1:E:1386:LYS:HA	1.71	0.71
1:B:436:PHE:HE1	1:B:438:SER:HB3	1.54	0.71
1:E:334:ARG:HG3	1:E:415:ILE:HD11	1.72	0.71
1:C:554:THR:HG22	1:C:556:ALA:H	1.55	0.71
1:A:1489:GLN:HE21	1:A:1492:GLN:HG3	1.56	0.70
1:D:1416:ASN:O	1:D:1420:ASN:HA	1.91	0.70
1:A:1919:ARG:HG2	1:B:998:ASN:ND2	2.06	0.70
1:C:867:TRP:HA	1:C:870:ILE:HD12	1.73	0.70
1:D:357:PHE:CZ	1:D:397:LYS:HG2	2.27	0.70
1:A:26:GLN:HG3	1:A:27:TYR:HA	1.73	0.70
1:A:1439:ILE:HG23	1:A:1450:ARG:HG3	1.74	0.70
1:A:1999:PHE:HE1	1:A:2003:HIS:CE1	2.09	0.70
1:B:1340:GLN:HB3	1:B:1355:HIS:HB2	1.73	0.70
1:D:2075:ALA:HA	1:D:2286:ARG:HH22	1.55	0.70
1:E:826:ASP:O	1:E:829:ASP:HB3	1.91	0.70
1:A:160:SER:HB3	1:A:982:LYS:HZ3	1.56	0.70
1:C:337:THR:HB	1:C:430:GLY:HA2	1.73	0.70
1:C:2250:ALA:HA	1:C:2253:MET:HE3	1.73	0.70
1:A:1437:ARG:HG3	1:A:1454:PHE:C	2.16	0.70
1:B:2102:GLN:HB3	1:B:2255:VAL:HG22	1.74	0.70
1:B:2437:LYS:HD2	1:B:2438:GLN:HB2	1.73	0.70
1:B:1437:ARG:NE	1:B:1455:PRO:HA	2.06	0.70
1:C:332:ILE:HD11	1:C:350:MET:HE1	1.72	0.70
1:D:26:GLN:HG3	1:D:27:TYR:HA	1.74	0.70
1:D:158:GLU:HG3	1:D:982:LYS:HG2	1.74	0.70
1:C:276:PHE:HA	1:C:281:TRP:CZ3	2.26	0.69
1:B:321:VAL:HG22	1:B:322:ASN:H	1.57	0.69
1:E:12:SER:HA	1:E:20:MET:HE1	1.74	0.69
1:B:367:ARG:HB2	1:B:390:LEU:HD21	1.72	0.69
1:D:2297:PHE:HE2	1:D:2328:TRP:HB2	1.57	0.69
1:B:1461:ILE:HG12	1:B:1463:ASN:H	1.58	0.69
1:E:2037:GLY:HA3	1:E:2326:GLY:HA2	1.75	0.69
1:A:349:LEU:HD21	1:A:356:GLN:HG3	1.73	0.69
1:A:404:ILE:HG21	1:A:414:LYS:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2469:CYS:HB3	1:D:2495:PRO:HA	1.73	0.69
1:A:1436:ARG:HE	1:A:1494:PHE:HD2	1.40	0.69
1:C:272:THR:HG23	1:C:275:ASN:H	1.56	0.69
1:C:334:ARG:HH21	1:C:342:LYS:HB3	1.57	0.69
1:C:1437:ARG:HH11	1:C:1453:GLU:HB2	1.58	0.69
1:E:554:THR:HG22	1:E:556:ALA:H	1.58	0.69
1:A:370:GLY:H	1:A:386:LEU:HB2	1.58	0.69
1:D:328:GLU:HB2	1:D:438:SER:HB2	1.74	0.69
1:E:610:THR:HG22	1:E:613:GLU:HG3	1.75	0.69
1:A:1365:GLY:H	1:A:1371:ARG:HG3	1.58	0.68
1:A:468:ILE:HD11	1:A:500:PHE:HZ	1.57	0.68
1:E:2102:GLN:HB3	1:E:2255:VAL:HG22	1.74	0.68
1:A:1437:ARG:HD3	1:A:1455:PRO:HG3	1.74	0.68
1:A:2516:ASP:H	1:A:2519:LYS:HB2	1.58	0.68
1:B:1649:LEU:HD12	1:B:1650:PRO:HD2	1.74	0.68
1:A:465:LEU:HA	1:A:468:ILE:HD12	1.75	0.68
1:A:587:ILE:HG12	1:A:593:VAL:HG21	1.75	0.68
1:A:964:ARG:HB3	1:A:976:GLN:NE2	2.09	0.68
1:D:236:LEU:HD13	1:D:487:PHE:HB2	1.75	0.68
1:D:2439:VAL:HG22	1:D:2532:ILE:HG13	1.75	0.68
1:D:1487:ASN:H	1:D:1489:GLN:HE22	1.41	0.68
1:A:347:PHE:HB3	1:A:415:ILE:HG23	1.75	0.68
1:B:2417:LEU:HA	1:B:2420:LEU:HD12	1.76	0.68
1:B:2469:CYS:HB3	1:B:2495:PRO:HA	1.75	0.68
1:D:70:ARG:HE	1:D:1880:MET:HG2	1.59	0.68
1:D:1395:ILE:HG22	1:D:1414:VAL:HG23	1.76	0.68
1:B:1626:LEU:HD12	1:B:1630:LEU:HD21	1.76	0.68
1:C:1049:ARG:H	1:C:1052:GLN:HE21	1.40	0.68
1:A:334:ARG:HH21	1:A:342:LYS:HB3	1.59	0.68
1:C:1639:ASP:HA	1:C:1832:TYR:HE2	1.58	0.68
1:A:826:ASP:O	1:A:829:ASP:HB3	1.94	0.68
1:A:998:ASN:ND2	1:E:1919:ARG:HG2	2.09	0.68
1:A:1852:CYS:HB3	1:A:1855:LEU:HD12	1.75	0.68
1:C:1675:GLU:OE1	1:C:1963:GLY:HA2	1.94	0.68
1:D:573:GLN:HA	1:D:576:LYS:HE2	1.76	0.68
1:A:1442:PRO:HD3	1:A:1451:LEU:HG	1.76	0.68
1:C:2102:GLN:HB3	1:C:2255:VAL:HG22	1.76	0.68
1:D:434:PHE:CZ	1:D:436:PHE:HB2	2.29	0.68
1:D:2120:ARG:HA	1:D:2237:MET:HE3	1.75	0.68
1:E:468:ILE:HG22	1:E:482:VAL:HG13	1.76	0.68
1:D:404:ILE:HG21	1:D:414:LYS:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLN:HG3	1:E:27:TYR:HA	1.76	0.67
1:E:680:LEU:HD12	1:E:684:ARG:HE	1.58	0.67
1:D:372:THR:HG23	1:D:386:LEU:HD11	1.76	0.67
1:C:1489:GLN:HG3	1:C:1492:GLN:HB2	1.77	0.67
1:B:273:PRO:HG2	1:B:442:THR:HG22	1.77	0.67
1:B:649:TRP:CD1	1:B:812:ARG:HH12	2.10	0.67
1:B:1172:GLU:HG3	1:B:1193:LYS:HD2	1.76	0.67
1:C:375:LYS:HG3	1:C:413:VAL:HG21	1.75	0.67
1:C:2423:PHE:HD2	1:C:2502:ASN:HD22	1.40	0.67
1:A:1921:LEU:HD13	1:A:1994:LEU:HD21	1.77	0.67
1:D:274:GLU:HB3	1:D:1405:TYR:HE1	1.59	0.67
1:D:760:PHE:CE1	1:D:764:MET:HE3	2.28	0.67
1:D:1764:MET:HE1	1:D:1769:ILE:HG13	1.77	0.67
1:E:2455:ALA:HB3	1:E:2474:LEU:HB3	1.75	0.67
1:E:545:SER:HA	1:E:586:THR:HA	1.77	0.67
1:E:1330:LEU:HD12	1:E:1331:THR:HG23	1.76	0.67
1:A:2102:GLN:HB3	1:A:2255:VAL:HG22	1.75	0.67
1:B:1812:MET:HE2	1:B:1812:MET:HA	1.77	0.67
1:C:1092:VAL:HG21	1:C:1109:PHE:HD1	1.60	0.67
1:C:1437:ARG:NH1	1:C:1453:GLU:HB2	2.08	0.67
1:D:1376:SER:HA	1:D:1379:LYS:HE3	1.76	0.67
1:E:332:ILE:HG22	1:E:334:ARG:HD2	1.77	0.67
1:D:2515:THR:HB	1:D:2516:ASP:CG	2.19	0.66
1:C:1367:GLY:HA2	1:C:1371:ARG:NE	2.10	0.66
1:B:824:GLY:O	1:B:827:THR:HB	1.96	0.66
1:B:14:THR:HB	1:B:20:MET:HB3	1.78	0.66
1:B:360:ARG:HD3	1:B:398:SER:HB2	1.77	0.66
1:B:573:GLN:HA	1:B:576:LYS:HE2	1.77	0.66
1:B:1675:GLU:OE1	1:B:1963:GLY:HA2	1.95	0.66
1:B:2064:LEU:HD11	1:B:2300:THR:HG21	1.78	0.66
1:C:129:LEU:HD11	1:C:1018:PHE:HE2	1.60	0.66
1:D:318:GLY:HA2	1:D:329:ALA:HA	1.77	0.66
1:B:1897:ARG:HG2	1:B:1916:TRP:CE2	2.31	0.66
1:C:436:PHE:HE1	1:C:438:SER:HB3	1.60	0.66
1:C:547:ASP:HB3	1:C:550:GLU:HB2	1.77	0.66
1:C:676:ILE:HA	1:C:679:LEU:HD12	1.76	0.66
1:C:2119:SER:HB3	1:D:2236:GLN:HG3	1.78	0.66
1:A:545:SER:HA	1:A:586:THR:HA	1.77	0.66
1:C:1241:LEU:HB2	1:C:1267:ILE:HG22	1.77	0.66
1:C:1919:ARG:HD2	1:D:998:ASN:HD21	1.60	0.66
1:D:1117:LEU:HD21	1:E:1205:ALA:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2102:GLN:HB3	1:D:2255:VAL:HG22	1.77	0.66
1:E:1410:GLY:HA3	1:E:1497:TYR:HE2	1.61	0.66
1:A:1720:HIS:HA	1:A:1766:GLN:NE2	2.11	0.66
1:B:1998:LEU:HD21	1:B:2002:ARG:HH21	1.61	0.66
1:C:235:LEU:HG	1:C:487:PHE:HZ	1.60	0.66
1:C:1764:MET:HE1	1:C:1769:ILE:HG13	1.77	0.66
1:E:545:SER:HB2	1:E:586:THR:HG22	1.76	0.66
1:A:637:PRO:HA	1:A:640:VAL:HG12	1.78	0.66
1:B:358:PHE:HB3	1:B:398:SER:HB3	1.78	0.66
1:D:2308:GLN:HA	1:D:2348:MET:HE1	1.76	0.66
1:A:710:ALA:HB2	1:E:2287:GLY:HA3	1.78	0.66
1:B:1167:HIS:HB3	1:B:1194:LEU:HD11	1.77	0.66
1:B:1965:VAL:HG12	1:B:1967:LYS:H	1.60	0.66
1:C:1439:ILE:HB	1:C:1483:VAL:HB	1.78	0.66
1:D:1461:ILE:HG12	1:D:1463:ASN:H	1.61	0.66
1:D:2455:ALA:HB3	1:D:2474:LEU:HB3	1.78	0.66
1:A:416:TYR:HD1	1:A:431:GLY:HA3	1.61	0.65
1:A:660:ILE:HA	1:A:663:LEU:HB2	1.78	0.65
1:A:1255:PHE:HB3	1:A:1281:LEU:HG	1.79	0.65
1:B:311:TYR:CZ	1:B:342:LYS:HD3	2.31	0.65
1:B:347:PHE:HB3	1:B:415:ILE:HD12	1.78	0.65
1:B:1376:SER:HA	1:B:1379:LYS:HG2	1.78	0.65
1:B:1880:MET:O	1:B:1883:LYS:HB2	1.94	0.65
1:C:1991:TRP:HB3	1:C:1995:ARG:HH12	1.61	0.65
1:B:219:ALA:HA	1:B:222:ARG:HE	1.61	0.65
1:C:112:MET:HG3	1:C:1979:PHE:HB2	1.76	0.65
1:C:321:VAL:HG22	1:C:322:ASN:H	1.62	0.65
1:E:349:LEU:HD13	1:E:356:GLN:NE2	2.10	0.65
1:D:412:GLY:HA3	1:D:434:PHE:HD2	1.60	0.65
1:A:2253:MET:HE2	1:E:2101:ILE:HD13	1.78	0.65
1:B:25:LEU:HA	1:B:27:TYR:HB2	1.79	0.65
1:C:198:PRO:HG2	1:C:245:GLU:HB3	1.78	0.65
1:D:272:THR:H	1:D:275:ASN:HD21	1.44	0.65
1:D:2053:MET:HA	1:D:2056:ARG:HG2	1.78	0.65
1:E:434:PHE:CZ	1:E:436:PHE:HB2	2.31	0.65
1:B:243:SER:H	1:B:246:LEU:HD12	1.61	0.65
1:B:1241:LEU:HB2	1:B:1267:ILE:HG22	1.77	0.65
1:C:1344:LYS:HA	1:C:1344:LYS:HE3	1.79	0.65
1:A:470:ARG:HD2	1:A:514:TYR:HE2	1.62	0.65
1:D:346:TYR:CZ	1:D:360:ARG:HB3	2.32	0.65
1:E:1399:VAL:HG22	1:E:1499:SER:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1162:PHE:CD2	1:C:1163:ARG:HG2	2.31	0.65
1:D:321:VAL:HG22	1:D:322:ASN:H	1.62	0.65
1:E:412:GLY:HA3	1:E:434:PHE:HD2	1.61	0.65
1:B:1675:GLU:HB3	1:B:1677:TRP:CD1	2.32	0.65
1:B:1855:LEU:HD12	1:B:1883:LYS:HG3	1.79	0.65
1:B:2423:PHE:HE1	1:B:2502:ASN:HB2	1.60	0.65
1:C:792:LEU:HA	1:C:867:TRP:HB3	1.79	0.65
1:C:1338:ILE:HG21	1:C:1354:LEU:HD22	1.79	0.65
1:C:1704:GLU:HG2	1:C:1780:LEU:HD13	1.78	0.65
1:C:2488:PHE:HB2	1:D:2485:MET:HE1	1.79	0.65
1:C:2356:ASP:HB3	1:D:2047:LEU:HD12	1.78	0.65
1:C:1373:LYS:HE2	1:C:1412:ILE:HB	1.79	0.64
1:D:1442:PRO:HD3	1:D:1451:LEU:HG	1.79	0.64
1:D:1991:TRP:HB3	1:D:1995:ARG:HH12	1.62	0.64
1:E:999:ARG:HA	1:E:1004:ILE:HD11	1.77	0.64
1:E:1316:PRO:HG2	1:E:1319:LEU:HD21	1.77	0.64
1:E:1720:HIS:HA	1:E:1766:GLN:NE2	2.13	0.64
1:E:587:ILE:HD11	1:E:593:VAL:HG11	1.79	0.64
1:E:2494:LEU:HD12	1:E:2495:PRO:HD2	1.80	0.64
1:A:1518:VAL:HG11	1:A:1553:ILE:HD13	1.78	0.64
1:C:2494:LEU:HD12	1:C:2495:PRO:HD2	1.80	0.64
1:D:446:LEU:O	1:D:450:LYS:HG2	1.98	0.64
1:E:368:GLU:OE2	1:E:420:TYR:HB2	1.97	0.64
1:E:1489:GLN:NE2	1:E:1492:GLN:HB2	2.13	0.64
1:A:67:ILE:HD11	1:A:89:SER:HA	1.77	0.64
1:C:350:MET:HG3	1:C:359:ILE:HG13	1.79	0.64
1:C:2184:ARG:HG2	1:C:2187:ALA:HB2	1.79	0.64
1:E:977:VAL:HB	1:E:981:ILE:HD13	1.78	0.64
1:A:1704:GLU:HG2	1:A:1780:LEU:HD13	1.79	0.64
1:B:1197:LEU:HD11	1:B:1201:GLY:HA2	1.79	0.64
1:B:1331:THR:HG23	1:B:1363:TYR:HD1	1.61	0.64
1:B:1919:ARG:HG2	1:C:998:ASN:ND2	2.12	0.64
1:C:235:LEU:HG	1:C:487:PHE:CZ	2.32	0.64
1:D:440:PRO:HB2	1:D:442:THR:HG23	1.78	0.64
1:A:219:ALA:HA	1:A:222:ARG:HE	1.63	0.64
1:A:2455:ALA:HB3	1:A:2474:LEU:HB2	1.80	0.64
1:C:129:LEU:HD13	1:C:1012:VAL:HG13	1.80	0.64
1:C:1316:PRO:HG2	1:C:1319:LEU:HD21	1.77	0.64
1:C:1638:ILE:H	1:C:1638:ILE:HD12	1.63	0.64
1:D:272:THR:H	1:D:275:ASN:ND2	1.96	0.64
1:D:2251:ALA:O	1:D:2254:GLN:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:LEU:HG	1:E:414:LYS:HD2	1.78	0.64
1:B:1555:ALA:HB1	1:B:1558:LEU:HD21	1.78	0.64
1:A:1167:HIS:HB3	1:A:1194:LEU:HD11	1.78	0.64
1:C:368:GLU:OE2	1:C:420:TYR:HB2	1.98	0.64
1:C:637:PRO:HA	1:C:640:VAL:HG12	1.78	0.64
1:C:1426:GLN:HB3	1:C:1461:ILE:HD13	1.79	0.64
1:D:2037:GLY:HA3	1:D:2326:GLY:HA2	1.79	0.64
1:B:1714:ALA:HB3	1:B:1717:TYR:HB2	1.80	0.64
1:C:2308:GLN:HA	1:C:2348:MET:HE1	1.80	0.64
1:E:158:GLU:OE1	1:E:982:LYS:HB3	1.97	0.64
1:B:1489:GLN:HG3	1:B:1492:GLN:HB2	1.80	0.63
1:C:1304:LYS:HG2	1:C:1602:PHE:HB3	1.79	0.63
1:D:1255:PHE:HB3	1:D:1281:LEU:HG	1.80	0.63
1:E:2250:ALA:HA	1:E:2253:MET:SD	2.38	0.63
1:C:2361:GLU:HB3	1:D:2484:PHE:CZ	2.32	0.63
1:E:792:LEU:HA	1:E:867:TRP:HB3	1.79	0.63
1:C:371:ALA:HA	1:C:382:ILE:HG23	1.79	0.63
1:D:198:PRO:HG2	1:D:245:GLU:HB3	1.79	0.63
1:D:676:ILE:HA	1:D:679:LEU:HD12	1.81	0.63
1:E:1371:ARG:O	1:E:1375:ILE:HG22	1.99	0.63
1:C:1425:VAL:HA	1:C:1463:ASN:HB3	1.80	0.63
1:A:328:GLU:HB3	1:A:330:TYR:HB3	1.80	0.63
1:B:1570:VAL:HA	1:B:1584:ILE:O	1.99	0.63
1:D:95:MET:O	1:D:95:MET:HE3	1.97	0.63
1:D:845:MET:HB3	1:D:847:LEU:HD23	1.79	0.63
1:A:1049:ARG:HB3	1:A:1872:ASP:OD2	1.98	0.63
1:A:1744:TYR:CE2	1:A:1746:ASP:HB2	2.34	0.63
1:C:1100:VAL:HB	1:C:1593:VAL:HG22	1.81	0.63
1:E:761:CYS:HA	1:E:764:MET:SD	2.39	0.63
1:E:2142:GLU:O	1:E:2146:MET:HG2	1.97	0.63
1:C:364:LYS:HD2	1:C:364:LYS:O	1.98	0.63
1:C:2109:VAL:HG23	1:C:2247:ARG:HH21	1.64	0.63
1:E:2289:LEU:HD13	1:E:2292:ILE:HD11	1.80	0.63
1:A:2031:VAL:HG12	1:B:779:ALA:HB3	1.80	0.63
1:B:311:TYR:CE1	1:B:342:LYS:HB3	2.34	0.63
1:B:867:TRP:HA	1:B:870:ILE:HD12	1.79	0.63
1:D:1540:SER:H	1:D:1544:MET:HE1	1.63	0.63
1:B:1053:THR:HG22	1:B:1055:MET:H	1.64	0.63
1:C:1714:ALA:HB3	1:C:1717:TYR:HB2	1.81	0.63
1:D:334:ARG:HH21	1:D:342:LYS:HB3	1.64	0.63
1:E:219:ALA:HA	1:E:222:ARG:HE	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LEU:HD11	1:A:765:ALA:HA	1.80	0.62
1:E:1135:LEU:HD11	1:E:1140:TRP:HE1	1.64	0.62
1:B:777:SER:HB3	1:B:2274:ARG:HE	1.64	0.62
1:E:501:ASP:HB2	1:E:522:HIS:CE1	2.35	0.62
1:E:1255:PHE:HB3	1:E:1281:LEU:HG	1.80	0.62
1:B:388:GLY:HA2	1:B:390:LEU:HD12	1.80	0.62
1:B:839:ASP:HA	1:B:849:ILE:HD13	1.81	0.62
1:C:387:SER:H	1:C:399:ASN:HB2	1.64	0.62
1:D:410:LYS:HA	1:D:436:PHE:O	1.99	0.62
1:D:1321:MET:HE3	1:D:1584:ILE:HG12	1.80	0.62
1:D:1639:ASP:HA	1:D:1832:TYR:HE2	1.63	0.62
1:A:483:LEU:HA	1:A:486:VAL:HG22	1.82	0.62
1:A:1633:ARG:HB2	1:A:1641:ILE:HD13	1.81	0.62
1:B:357:PHE:CZ	1:B:397:LYS:HG2	2.34	0.62
1:C:1287:LEU:HD11	1:C:1309:PHE:HB2	1.81	0.62
1:D:346:TYR:CE2	1:D:360:ARG:HB3	2.35	0.62
1:B:792:LEU:HA	1:B:867:TRP:HB3	1.80	0.62
1:C:310:ALA:HB2	1:C:317:THR:HB	1.81	0.62
1:C:761:CYS:O	1:C:764:MET:HB2	2.00	0.62
1:D:1100:VAL:HB	1:D:1593:VAL:HG22	1.82	0.62
1:A:112:MET:HG3	1:A:1979:PHE:HB2	1.80	0.62
1:A:1999:PHE:CE1	1:A:2003:HIS:CE1	2.87	0.62
1:B:276:PHE:HA	1:B:281:TRP:CZ3	2.34	0.62
1:B:1368:ASN:HB2	1:B:1370:ILE:HG22	1.81	0.62
1:B:2455:ALA:HB3	1:B:2474:LEU:HB3	1.82	0.62
1:E:276:PHE:HA	1:E:281:TRP:CE3	2.35	0.62
1:A:321:VAL:HG11	1:A:352:GLU:HA	1.82	0.62
1:D:235:LEU:HG	1:D:487:PHE:CZ	2.35	0.62
1:D:959:VAL:HG13	1:D:961:LEU:HD22	1.81	0.62
1:E:1304:LYS:HG2	1:E:1602:PHE:HB3	1.80	0.62
1:A:680:LEU:HD13	1:A:684:ARG:HH21	1.65	0.62
1:A:1991:TRP:HB3	1:A:1995:ARG:HH12	1.65	0.62
1:B:1363:TYR:HB3	1:B:1375:ILE:HD11	1.81	0.62
1:B:1720:HIS:HA	1:B:1766:GLN:NE2	2.14	0.62
1:D:1410:GLY:HA3	1:D:1497:TYR:HE2	1.65	0.62
1:A:337:THR:HB	1:A:430:GLY:HA2	1.82	0.62
1:A:1426:GLN:HG3	1:A:1463:ASN:OD1	1.99	0.62
1:B:528:ASN:HD21	1:B:536:ILE:HG21	1.62	0.62
1:C:1855:LEU:HD12	1:C:1883:LYS:HG3	1.81	0.62
1:C:2031:VAL:HG12	1:D:779:ALA:HB3	1.81	0.62
1:A:954:ILE:HG22	1:A:956:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1049:ARG:H	1:C:1052:GLN:NE2	1.96	0.62
1:D:235:LEU:HG	1:D:487:PHE:HZ	1.64	0.62
1:D:1049:ARG:HG3	1:D:1872:ASP:OD2	2.00	0.62
1:E:776:LEU:HD11	1:E:814:HIS:HB2	1.81	0.62
1:A:129:LEU:HD13	1:A:1012:VAL:HG13	1.82	0.61
1:B:7:LEU:HA	1:B:10:LYS:HD3	1.81	0.61
1:C:296:TYR:CZ	1:C:462:PRO:HG3	2.35	0.61
1:D:373:LEU:HD23	1:D:381:GLY:H	1.63	0.61
1:D:1046:PRO:O	1:D:1812:MET:HE1	1.99	0.61
1:D:1243:VAL:HG23	1:D:1265:MET:HB3	1.82	0.61
1:E:1046:PRO:HG2	1:E:1889:ARG:HH11	1.65	0.61
1:E:1340:GLN:HB3	1:E:1355:HIS:HB2	1.82	0.61
1:B:761:CYS:HA	1:B:764:MET:HE2	1.82	0.61
1:B:1519:MET:HB2	1:B:1568:ASP:OD1	2.00	0.61
1:E:370:GLY:H	1:E:386:LEU:HB2	1.65	0.61
1:E:505:VAL:HG11	1:E:598:TYR:HD2	1.66	0.61
1:A:1230:LEU:HA	1:A:1244:PHE:O	1.99	0.61
1:A:1644:MET:HG3	1:A:1848:TRP:CE2	2.35	0.61
1:E:679:LEU:HB2	1:E:711:THR:HG21	1.83	0.61
1:E:2100:ARG:HH21	1:E:2104:ARG:HH21	1.47	0.61
1:A:168:LEU:O	1:A:171:GLU:HG3	2.01	0.61
1:A:2515:THR:HB	1:A:2516:ASP:CG	2.25	0.61
1:B:357:PHE:CE2	1:B:397:LYS:HE3	2.36	0.61
1:C:29:SER:HB2	1:C:1015:ARG:HA	1.82	0.61
1:D:2074:MET:HE1	1:D:2289:LEU:HG	1.82	0.61
1:E:14:THR:HB	1:E:20:MET:HB3	1.82	0.61
1:E:663:LEU:HD21	1:E:769:LEU:HD22	1.82	0.61
1:E:1197:LEU:HD11	1:E:1201:GLY:HA2	1.81	0.61
1:E:1998:LEU:HD11	1:E:2002:ARG:HH11	1.66	0.61
1:D:66:ARG:HH21	1:D:1878:ASP:HB3	1.65	0.61
1:D:112:MET:HG3	1:D:1979:PHE:HB2	1.82	0.61
1:E:1100:VAL:HB	1:E:1593:VAL:HG22	1.83	0.61
1:E:2123:ALA:HB3	1:E:2237:MET:HE1	1.83	0.61
1:A:87:SER:HA	1:A:90:ARG:HD3	1.83	0.61
1:A:332:ILE:HG22	1:A:334:ARG:HD2	1.81	0.61
1:A:367:ARG:HD3	1:A:390:LEU:HD21	1.82	0.61
1:A:2251:ALA:O	1:A:2254:GLN:HG3	2.01	0.61
1:C:1639:ASP:HA	1:C:1832:TYR:CE2	2.36	0.61
1:D:1749:LYS:HB3	1:D:1751:GLN:HG2	1.83	0.61
1:D:2308:GLN:NE2	1:D:2321:THR:HA	2.15	0.61
1:E:867:TRP:HA	1:E:870:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1518:VAL:HG11	1:E:1553:ILE:HD13	1.83	0.61
1:A:1919:ARG:HG2	1:B:998:ASN:HD21	1.65	0.61
1:B:1362:ARG:NH2	1:B:1363:TYR:HB2	2.16	0.61
1:B:1399:VAL:HG22	1:B:1499:SER:HA	1.83	0.61
1:C:595:SER:O	1:C:599:ARG:HG3	2.00	0.61
1:E:1415:TYR:HE1	1:E:1473:THR:HG22	1.66	0.61
1:E:1991:TRP:HB3	1:E:1995:ARG:HH12	1.66	0.61
1:A:2515:THR:HB	1:A:2516:ASP:OD1	2.00	0.61
1:C:1169:ILE:HD13	1:C:1194:LEU:HB2	1.83	0.61
1:A:1437:ARG:HH11	1:A:1453:GLU:HB2	1.66	0.61
1:C:321:VAL:HG21	1:C:352:GLU:HG2	1.81	0.61
1:D:602:LEU:HD23	1:D:605:ARG:HD3	1.83	0.61
1:E:224:PRO:HA	1:E:227:MET:HB2	1.83	0.61
1:E:1436:ARG:HB2	1:E:1485:GLY:HA2	1.83	0.61
1:E:1508:GLY:C	1:E:1576:LYS:HE3	2.26	0.61
1:B:11:ILE:HD11	1:B:41:LEU:HD23	1.83	0.60
1:A:198:PRO:HG2	1:A:245:GLU:HB3	1.82	0.60
1:A:1540:SER:H	1:A:1544:MET:HE1	1.65	0.60
1:A:2053:MET:HE1	1:A:2306:MET:HB2	1.83	0.60
1:A:2239:ALA:O	1:A:2242:GLU:HG3	2.00	0.60
1:B:1255:PHE:HB3	1:B:1281:LEU:HG	1.82	0.60
1:B:2099:ILE:HD13	1:B:2258:GLN:HB3	1.81	0.60
1:C:2410:GLN:HB3	1:C:2512:PRO:HA	1.83	0.60
1:D:2026:LEU:HD21	1:E:818:ASN:HB3	1.82	0.60
1:E:1890:LEU:O	1:E:1893:GLN:HG2	2.00	0.60
1:E:2436:LEU:HD12	1:E:2501:VAL:HA	1.82	0.60
1:A:1516:ILE:HD11	1:A:1569:ILE:HG23	1.83	0.60
1:B:999:ARG:HG2	1:B:1004:ILE:HD11	1.83	0.60
1:C:330:TYR:HB2	1:C:436:PHE:CZ	2.36	0.60
1:A:1162:PHE:CG	1:A:1241:LEU:HD21	2.36	0.60
1:A:1662:PHE:HZ	1:A:1725:LEU:HD13	1.67	0.60
1:C:901:ALA:N	1:C:907:SER:HB3	2.13	0.60
1:C:1371:ARG:HG3	1:C:1372:ASN:H	1.66	0.60
1:A:298:GLY:HA3	1:A:315:ILE:HG23	1.83	0.60
1:B:95:MET:HE1	1:B:1968:ASN:HB3	1.82	0.60
1:B:250:LEU:HD11	1:B:454:LEU:HB2	1.82	0.60
1:B:501:ASP:HB3	1:B:522:HIS:CE1	2.37	0.60
1:B:910:PRO:HB3	1:B:914:GLU:HG3	1.83	0.60
1:C:692:ALA:HA	1:C:741:MET:HE3	1.82	0.60
1:C:1162:PHE:CG	1:C:1241:LEU:HD21	2.37	0.60
1:E:321:VAL:HG22	1:E:322:ASN:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:LYS:HG2	1:E:453:ARG:HH22	1.67	0.60
1:A:321:VAL:HG22	1:A:322:ASN:H	1.66	0.60
1:A:1691:ARG:HH22	1:A:1733:THR:HG21	1.66	0.60
1:A:1993:THR:O	1:A:1997:ARG:HG2	2.00	0.60
1:A:2184:ARG:HH12	1:E:2184:ARG:HH12	1.48	0.60
1:A:2457:LEU:HD12	1:A:2507:LEU:HD21	1.84	0.60
1:B:28:LEU:HD12	1:B:32:GLU:HB3	1.82	0.60
1:B:1633:ARG:HG3	1:B:1640:THR:HG22	1.83	0.60
1:C:2469:CYS:HB3	1:C:2495:PRO:HA	1.82	0.60
1:D:1804:GLU:HA	1:D:1808:TYR:HB2	1.83	0.60
1:A:792:LEU:HA	1:A:867:TRP:HB3	1.84	0.60
1:B:954:ILE:HG22	1:B:956:PRO:HD3	1.84	0.60
1:C:67:ILE:HD11	1:C:89:SER:HA	1.82	0.60
1:D:663:LEU:HD21	1:D:769:LEU:HD22	1.84	0.60
1:A:352:GLU:N	1:A:357:PHE:HZ	2.00	0.60
1:B:2341:LEU:O	1:B:2345:LEU:HG	2.01	0.60
1:C:206:ILE:HD13	1:C:922:MET:HE3	1.83	0.60
1:C:954:ILE:HG22	1:C:956:PRO:HD3	1.84	0.60
1:D:206:ILE:HG23	1:D:922:MET:HE3	1.82	0.60
1:A:437:GLU:HB2	1:A:439:TYR:CE2	2.36	0.60
1:C:201:GLN:HA	1:C:204:GLU:OE2	2.02	0.60
1:D:218:SER:O	1:D:221:SER:HB3	2.02	0.60
1:D:345:ASN:HB3	1:D:346:TYR:HB2	1.83	0.60
1:A:384:GLY:HA3	1:A:401:LEU:HD11	1.84	0.60
1:A:1416:ASN:O	1:A:1420:ASN:CA	2.43	0.60
1:B:780:GLU:HA	1:B:828:LEU:HD21	1.83	0.60
1:D:2360:LEU:HD11	1:E:2472:ILE:HA	1.83	0.60
1:B:1246:TYR:HB3	1:B:1262:VAL:HG22	1.84	0.59
1:C:587:ILE:HG12	1:C:593:VAL:HG21	1.83	0.59
1:C:1902:TYR:HE2	1:C:2007:ILE:HB	1.67	0.59
1:D:728:ASP:HB2	1:D:737:ILE:HG12	1.83	0.59
1:D:839:ASP:HA	1:D:849:ILE:HD13	1.82	0.59
1:D:1367:GLY:HA2	1:D:1371:ARG:NE	2.11	0.59
1:A:1523:LYS:HZ1	1:A:1556:SER:H	1.49	0.59
1:A:2026:LEU:HD21	1:B:818:ASN:HB3	1.84	0.59
1:C:1749:LYS:HB2	1:C:1751:GLN:HG2	1.84	0.59
1:D:708:ILE:O	1:D:712:LEU:HB3	2.02	0.59
1:D:1304:LYS:HG2	1:D:1602:PHE:HB3	1.84	0.59
1:E:1570:VAL:HA	1:E:1584:ILE:O	2.02	0.59
1:A:331:LYS:O	1:A:436:PHE:HA	2.02	0.59
1:A:2151:ALA:O	1:A:2155:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:ILE:O	1:C:712:LEU:HB3	2.02	0.59
1:D:2465:MET:HG2	1:D:2466:PRO:HD2	1.83	0.59
1:E:777:SER:HB3	1:E:2274:ARG:HD2	1.83	0.59
1:A:308:THR:HG21	1:A:359:ILE:HD11	1.83	0.59
1:C:6:VAL:O	1:C:10:LYS:HG3	2.01	0.59
1:C:899:VAL:HG11	1:C:904:LYS:HD2	1.84	0.59
1:C:1230:LEU:HA	1:C:1244:PHE:O	2.03	0.59
1:C:2051:PRO:HA	1:C:2054:LEU:HD12	1.83	0.59
1:D:2454:ARG:NH2	1:D:2513:ASP:HB3	2.18	0.59
1:A:292:GLU:OE2	1:A:293:VAL:HG13	2.02	0.59
1:D:680:LEU:HB3	1:D:684:ARG:HE	1.66	0.59
1:D:1162:PHE:CG	1:D:1241:LEU:HD21	2.38	0.59
1:D:1666:LYS:HE2	1:D:1703:SER:HA	1.85	0.59
1:D:2198:LEU:HA	1:D:2201:THR:HG22	1.84	0.59
1:E:367:ARG:HD3	1:E:390:LEU:HD21	1.84	0.59
1:A:547:ASP:HB3	1:A:550:GLU:HB2	1.85	0.59
1:B:1439:ILE:HA	1:B:1452:PHE:O	2.02	0.59
1:C:104:VAL:HG11	1:C:110:ALA:HB3	1.83	0.59
1:D:173:ILE:HD11	1:D:950:PHE:HD1	1.67	0.59
1:D:587:ILE:HD11	1:D:593:VAL:HG11	1.85	0.59
1:D:1879:PRO:O	1:D:1882:TYR:HB2	2.03	0.59
1:E:1675:GLU:HB3	1:E:1677:TRP:CD1	2.38	0.59
1:A:2454:ARG:NH2	1:A:2513:ASP:HB3	2.17	0.59
1:C:1633:ARG:HB2	1:C:1641:ILE:HD13	1.85	0.59
1:C:2094:LEU:HD21	1:D:2264:HIS:HE1	1.68	0.59
1:E:1162:PHE:CG	1:E:1241:LEU:HD21	2.37	0.59
1:E:1890:LEU:HA	1:E:1893:GLN:OE1	2.02	0.59
1:A:2118:GLU:OE2	1:B:2236:GLN:HG2	2.03	0.59
1:A:2350:LYS:HD3	1:B:2299:LEU:HD13	1.83	0.59
1:B:1437:ARG:HE	1:B:1455:PRO:HA	1.67	0.59
1:B:2515:THR:HB	1:B:2516:ASP:CG	2.27	0.59
1:C:1197:LEU:HD11	1:C:1201:GLY:HA2	1.85	0.59
1:D:353:GLY:HA3	1:D:397:LYS:HD2	1.85	0.59
1:D:1704:GLU:HG2	1:D:1780:LEU:HD13	1.84	0.59
1:D:2149:LEU:HD23	1:D:2209:LYS:HB3	1.85	0.59
1:B:27:TYR:HB3	1:B:28:LEU:HD22	1.84	0.59
1:B:236:LEU:HB2	1:B:487:PHE:CG	2.38	0.59
1:C:1675:GLU:HB3	1:C:1677:TRP:CD1	2.38	0.59
1:E:11:ILE:HD11	1:E:41:LEU:HD23	1.85	0.59
1:A:1437:ARG:NH1	1:A:1453:GLU:HB2	2.17	0.59
1:C:1323:SER:HA	1:C:1334:GLU:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LEU:HB3	1:B:789:PHE:CE1	2.37	0.58
1:B:1839:TYR:CZ	1:B:1851:ASN:HB2	2.38	0.58
1:D:355:ASN:ND2	1:D:402:SER:HB3	2.18	0.58
1:D:792:LEU:HA	1:D:867:TRP:HB3	1.85	0.58
1:D:1487:ASN:H	1:D:1489:GLN:NE2	2.01	0.58
1:D:2115:VAL:HG22	1:E:2239:ALA:HB1	1.85	0.58
1:A:276:PHE:HA	1:A:281:TRP:CZ3	2.38	0.58
1:D:2435:GLN:HG3	1:D:2437:LYS:NZ	2.18	0.58
1:E:25:LEU:HA	1:E:27:TYR:HB2	1.84	0.58
1:A:2494:LEU:HD12	1:A:2495:PRO:HD2	1.84	0.58
1:B:76:SER:HB3	1:B:80:ARG:HE	1.68	0.58
1:B:2500:SER:HB3	1:B:2503:ASP:HB2	1.85	0.58
1:C:278:SER:HB3	1:C:281:TRP:HB3	1.84	0.58
1:D:158:GLU:HG3	1:D:982:LYS:HE3	1.84	0.58
1:D:1570:VAL:HA	1:D:1584:ILE:O	2.04	0.58
1:D:2423:PHE:HD2	1:D:2502:ASN:HD22	1.48	0.58
1:A:360:ARG:HB3	1:A:396:PHE:H	1.68	0.58
1:B:2046:SER:HB3	1:B:2306:MET:HG2	1.86	0.58
1:C:464:GLU:HG2	1:C:500:PHE:CD2	2.39	0.58
1:C:475:GLN:HB2	1:C:477:ILE:HG12	1.85	0.58
1:C:1150:VAL:HG12	1:C:1152:PRO:HD3	1.84	0.58
1:D:665:THR:HG23	1:D:667:GLU:H	1.67	0.58
1:E:708:ILE:HG21	1:E:724:LEU:HD21	1.84	0.58
1:A:999:ARG:HA	1:A:1004:ILE:HD11	1.85	0.58
1:A:1519:MET:HB2	1:A:1568:ASP:OD1	2.03	0.58
1:C:168:LEU:O	1:C:171:GLU:HG3	2.04	0.58
1:C:899:VAL:HG11	1:C:904:LYS:HB2	1.85	0.58
1:C:2277:THR:HA	1:C:2281:LEU:HD23	1.84	0.58
1:D:14:THR:HA	1:D:20:MET:HE2	1.83	0.58
1:D:324:GLU:HB3	1:D:351:TYR:CD2	2.39	0.58
1:D:817:ILE:HA	1:D:820:LEU:HG	1.85	0.58
1:D:1426:GLN:HE21	1:D:1461:ILE:HG21	1.69	0.58
1:D:1439:ILE:HD13	1:D:1453:GLU:HA	1.86	0.58
1:E:1516:ILE:HD11	1:E:1569:ILE:HG23	1.86	0.58
1:A:1523:LYS:NZ	1:A:1556:SER:H	2.00	0.58
1:B:2297:PHE:CE2	1:B:2328:TRP:HB2	2.38	0.58
1:C:1442:PRO:HD3	1:C:1451:LEU:HG	1.84	0.58
1:C:1519:MET:HB2	1:C:1568:ASP:OD1	2.04	0.58
1:E:954:ILE:HG22	1:E:956:PRO:HD3	1.86	0.58
1:B:1162:PHE:CG	1:B:1241:LEU:HD21	2.38	0.58
1:E:450:LYS:HG2	1:E:453:ARG:NH2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1804:GLU:HA	1:E:1808:TYR:HB2	1.86	0.58
1:A:288:LEU:HB3	1:A:292:GLU:OE2	2.03	0.58
1:B:1376:SER:HA	1:B:1379:LYS:HE3	1.86	0.58
1:B:2129:LYS:HD3	1:C:2225:ILE:HG22	1.85	0.58
1:C:339:ASP:OD2	1:C:343:ASN:HB2	2.04	0.58
1:C:839:ASP:HA	1:C:849:ILE:HD13	1.85	0.58
1:D:1150:VAL:HG12	1:D:1152:PRO:HD3	1.85	0.58
1:E:2368:LEU:HD22	1:E:2528:ILE:HB	1.86	0.58
1:D:628:THR:HA	1:D:631:LEU:HG	1.86	0.58
1:D:1411:PRO:HA	1:D:1425:VAL:O	2.02	0.58
1:D:2494:LEU:HD12	1:D:2495:PRO:HD2	1.85	0.58
1:E:356:GLN:HE22	1:E:409:TYR:HB2	1.68	0.58
1:E:1998:LEU:O	1:E:2002:ARG:HG2	2.03	0.58
1:B:217:LEU:HB3	1:B:220:LEU:HB3	1.86	0.58
1:B:784:LEU:HB3	1:B:789:PHE:HE1	1.69	0.58
1:B:1287:LEU:HD11	1:B:1309:PHE:HB2	1.85	0.58
1:C:1399:VAL:HA	1:C:1498:GLN:O	2.03	0.58
1:A:2356:ASP:HB3	1:B:2047:LEU:HD12	1.86	0.57
1:B:320:VAL:HG22	1:B:327:LEU:HA	1.86	0.57
1:B:2417:LEU:HD21	1:B:2507:LEU:HG	1.86	0.57
1:D:126:ALA:HA	1:D:129:LEU:HD23	1.85	0.57
1:D:2184:ARG:HE	1:D:2190:ARG:HH21	1.52	0.57
1:E:198:PRO:HG2	1:E:245:GLU:HB3	1.86	0.57
1:E:1409:GLY:HA3	1:E:1427:GLY:HA3	1.86	0.57
1:A:126:ALA:HA	1:A:129:LEU:HD23	1.86	0.57
1:A:321:VAL:HG21	1:A:352:GLU:HG2	1.85	0.57
1:B:235:LEU:HD23	1:B:487:PHE:HZ	1.68	0.57
1:B:1230:LEU:HA	1:B:1244:PHE:O	2.04	0.57
1:C:1135:LEU:HD11	1:C:1140:TRP:HE1	1.69	0.57
1:C:2436:LEU:HD11	1:C:2499:ILE:HD12	1.86	0.57
1:D:26:GLN:CG	1:D:27:TYR:HA	2.34	0.57
1:D:528:ASN:HD21	1:D:536:ILE:HG21	1.69	0.57
1:D:1378:MET:HE1	1:D:1393:PHE:CG	2.40	0.57
1:E:276:PHE:CD1	1:E:441:LEU:HD21	2.39	0.57
1:A:33:LEU:HA	1:A:36:ILE:HG22	1.86	0.57
1:A:334:ARG:HD3	1:A:334:ARG:H	1.69	0.57
1:A:1197:LEU:HD12	1:A:1203:TRP:CZ2	2.39	0.57
1:B:760:PHE:CD2	1:B:764:MET:HE1	2.39	0.57
1:E:236:LEU:HD22	1:E:487:PHE:HB2	1.86	0.57
1:E:1371:ARG:HG3	1:E:1372:ASN:N	2.19	0.57
1:A:2500:SER:HB3	1:A:2503:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ILE:HD11	1:B:593:VAL:HG11	1.87	0.57
1:B:1049:ARG:HB2	1:B:1872:ASP:OD1	2.03	0.57
1:D:1096:TYR:HD1	1:D:1306:SER:HB2	1.69	0.57
1:E:1665:PRO:HA	1:E:1704:GLU:OE1	2.03	0.57
1:A:217:LEU:HB3	1:A:220:LEU:HB3	1.86	0.57
1:A:977:VAL:HG12	1:E:2002:ARG:HA	1.86	0.57
1:A:1481:TYR:HE1	1:A:1498:GLN:HE22	1.53	0.57
1:A:2327:ALA:HB1	1:A:2337:ALA:HB1	1.85	0.57
1:B:1049:ARG:H	1:B:1052:GLN:HE21	1.51	0.57
1:C:25:LEU:HA	1:C:27:TYR:HB2	1.87	0.57
1:C:1431:ASN:HD21	1:C:1434:TYR:HB2	1.68	0.57
1:C:1451:LEU:HD12	1:C:1479:CYS:SG	2.44	0.57
1:D:824:GLY:O	1:D:827:THR:HB	2.03	0.57
1:E:1305:ALA:HB3	1:E:1601:LEU:HD21	1.87	0.57
1:E:1415:TYR:CE1	1:E:1473:THR:HG22	2.40	0.57
1:A:1804:GLU:HA	1:A:1808:TYR:HB2	1.84	0.57
1:B:321:VAL:HG21	1:B:352:GLU:HG2	1.86	0.57
1:B:347:PHE:HB3	1:B:415:ILE:HG23	1.85	0.57
1:B:1130:MET:HG3	1:B:1132:ALA:H	1.69	0.57
1:B:1399:VAL:HG13	1:B:1497:TYR:HB3	1.87	0.57
1:B:1749:LYS:HB2	1:B:1751:GLN:HG2	1.87	0.57
1:C:2178:LEU:HD21	1:D:2178:LEU:HD13	1.86	0.57
1:D:129:LEU:HD11	1:D:1018:PHE:HE2	1.68	0.57
1:D:1626:LEU:H	1:D:1626:LEU:HD23	1.69	0.57
1:E:279:GLN:HE22	1:E:297:LEU:HD11	1.70	0.57
1:E:2434:ARG:HB2	1:E:2501:VAL:HG11	1.85	0.57
1:B:279:GLN:O	1:B:282:ILE:HG22	2.04	0.57
1:B:683:LEU:HD21	1:B:707:PHE:HB3	1.86	0.57
1:B:1810:PRO:HA	1:B:1829:TRP:HE1	1.70	0.57
1:C:416:TYR:HD1	1:C:431:GLY:HA3	1.68	0.57
1:D:328:GLU:CB	1:D:438:SER:HB2	2.33	0.57
1:D:547:ASP:HB3	1:D:550:GLU:HB2	1.86	0.57
1:D:1644:MET:HG3	1:D:1848:TRP:CE2	2.40	0.57
1:E:1626:LEU:HD23	1:E:1626:LEU:H	1.69	0.57
1:A:181:SER:O	1:A:185:MET:HG2	2.05	0.57
1:C:357:PHE:CE2	1:C:397:LYS:HA	2.40	0.57
1:D:1571:PHE:HB2	1:D:1584:ILE:HB	1.87	0.57
1:D:1633:ARG:HB2	1:D:1641:ILE:HD13	1.86	0.57
1:D:2064:LEU:HD13	1:D:2296:PHE:HD2	1.69	0.57
1:E:226:VAL:HG12	1:E:876:TRP:CD1	2.39	0.57
1:A:349:LEU:HD22	1:A:409:TYR:CG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:SER:O	1:A:772:GLN:HG2	2.04	0.57
1:A:1123:ARG:HD2	1:A:1143:TRP:CH2	2.40	0.57
1:A:1150:VAL:HG12	1:A:1152:PRO:HD3	1.87	0.57
1:B:1304:LYS:HG2	1:B:1602:PHE:HB3	1.86	0.57
1:B:2056:ARG:HA	1:B:2059:ASN:HD21	1.69	0.57
1:C:856:MET:SD	1:C:861:VAL:HG23	2.44	0.57
1:D:545:SER:HB2	1:D:586:THR:HG22	1.85	0.57
1:D:2328:TRP:CD2	1:D:2334:GLY:HA3	2.39	0.57
1:A:25:LEU:HA	1:A:27:TYR:HB2	1.86	0.57
1:A:2129:LYS:NZ	1:A:2133:LEU:HB2	2.20	0.57
1:B:1175:GLU:HG2	1:B:1175:GLU:O	2.05	0.57
1:B:1419:LYS:HB3	1:B:1421:TYR:CE1	2.40	0.57
1:B:1641:ILE:HG22	1:B:1642:LEU:HD23	1.86	0.57
1:B:2115:VAL:HG22	1:C:2239:ALA:HB1	1.86	0.57
1:C:318:GLY:HA2	1:C:329:ALA:HA	1.87	0.57
1:C:1439:ILE:HG23	1:C:1450:ARG:HG3	1.87	0.57
1:D:289:GLU:O	1:D:292:GLU:HG3	2.05	0.57
1:E:172:HIS:HA	1:E:175:ARG:HH12	1.68	0.57
1:A:584:GLN:HG2	1:A:586:THR:HG23	1.87	0.56
1:C:545:SER:HA	1:C:586:THR:HA	1.87	0.56
1:D:388:GLY:HA2	1:D:390:LEU:HD12	1.87	0.56
1:D:443:ILE:HA	1:D:446:LEU:HD12	1.86	0.56
1:A:350:MET:HB2	1:A:359:ILE:HA	1.87	0.56
1:B:226:VAL:HG12	1:B:876:TRP:CE3	2.41	0.56
1:C:2383:THR:HA	1:C:2386:LEU:HD12	1.84	0.56
1:D:67:ILE:HD11	1:D:89:SER:HA	1.87	0.56
1:D:984:THR:HG23	1:D:987:ALA:H	1.70	0.56
1:E:349:LEU:HD22	1:E:356:GLN:HG2	1.86	0.56
1:A:357:PHE:CE2	1:A:397:LYS:HA	2.40	0.56
1:A:848:ASP:HB3	1:A:851:MET:HG2	1.85	0.56
1:A:1744:TYR:HE2	1:A:1746:ASP:HB2	1.70	0.56
1:A:2267:ALA:O	1:A:2270:GLU:HG3	2.05	0.56
1:B:8:LEU:HD23	1:B:20:MET:O	2.05	0.56
1:B:26:GLN:CG	1:B:27:TYR:HA	2.33	0.56
1:B:412:GLY:HA3	1:B:434:PHE:HD2	1.70	0.56
1:B:959:VAL:HG13	1:B:961:LEU:HD22	1.86	0.56
1:B:1902:TYR:CD1	1:B:2007:ILE:HD13	2.40	0.56
1:C:14:THR:HA	1:C:20:MET:HE2	1.88	0.56
1:C:1123:ARG:HD2	1:C:1143:TRP:CH2	2.40	0.56
1:C:1436:ARG:HB2	1:C:1485:GLY:HA2	1.86	0.56
1:C:2437:LYS:HD2	1:C:2438:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LEU:HD22	1:D:409:TYR:HD1	1.71	0.56
1:A:410:LYS:HD3	1:A:436:PHE:HD1	1.71	0.56
1:A:679:LEU:HD13	1:A:711:THR:HG21	1.87	0.56
1:B:345:ASN:HD22	1:B:364:LYS:HE3	1.70	0.56
1:D:348:ASP:N	1:D:359:ILE:HG22	2.21	0.56
1:A:2126:ARG:HD3	1:B:2229:ASN:HD21	1.70	0.56
1:B:350:MET:HE3	1:B:395:ASN:OD1	2.05	0.56
1:B:1394:ILE:HG12	1:B:1417:LYS:HZ2	1.70	0.56
1:B:1629:GLN:HG2	1:B:1649:LEU:HD11	1.87	0.56
1:B:1644:MET:HG3	1:B:1848:TRP:CE2	2.40	0.56
1:D:331:LYS:HB2	1:D:444:PHE:HE2	1.70	0.56
1:D:498:LEU:HD12	1:D:502:ASP:OD2	2.05	0.56
1:E:226:VAL:HG21	1:E:879:VAL:HG21	1.87	0.56
1:E:235:LEU:HD23	1:E:487:PHE:HZ	1.70	0.56
1:A:274:GLU:HB3	1:A:1405:TYR:HE1	1.70	0.56
1:A:330:TYR:HB2	1:A:436:PHE:CE2	2.41	0.56
1:A:349:LEU:HD22	1:A:409:TYR:CD1	2.40	0.56
1:A:1815:GLN:HG2	1:A:1889:ARG:HH12	1.70	0.56
1:B:465:LEU:HA	1:B:468:ILE:HG12	1.87	0.56
1:C:969:SER:O	1:C:972:LEU:HD22	2.05	0.56
1:C:1436:ARG:HE	1:C:1494:PHE:HD2	1.53	0.56
1:C:1555:ALA:HB1	1:C:1558:LEU:HD21	1.87	0.56
1:C:1846:ALA:HB1	1:C:1848:TRP:CE2	2.41	0.56
1:C:2438:GLN:HB3	1:C:2533:ARG:HB2	1.86	0.56
1:D:276:PHE:CD1	1:D:281:TRP:HZ3	2.24	0.56
1:D:348:ASP:C	1:D:359:ILE:HG22	2.30	0.56
1:D:489:THR:HA	1:D:503:ALA:HB1	1.87	0.56
1:A:1162:PHE:CD1	1:A:1241:LEU:HD21	2.41	0.56
1:B:1632:SER:HA	1:C:1164:GLU:HG3	1.88	0.56
1:C:11:ILE:HD11	1:C:41:LEU:HD23	1.88	0.56
1:C:1167:HIS:HB3	1:C:1194:LEU:HD11	1.87	0.56
1:D:256:GLU:HA	1:D:259:ALA:HB2	1.88	0.56
1:D:664:CYS:SG	1:D:803:ASN:HA	2.46	0.56
1:E:181:SER:O	1:E:185:MET:HG2	2.05	0.56
1:E:1363:TYR:HB3	1:E:1375:ILE:HD11	1.86	0.56
1:E:1367:GLY:HA2	1:E:1371:ARG:NE	2.11	0.56
1:A:1456:PHE:CD1	1:A:1461:ILE:HD13	2.41	0.56
1:B:11:ILE:HA	1:B:40:GLN:NE2	2.21	0.56
1:B:1879:PRO:O	1:B:1882:TYR:HB2	2.06	0.56
1:B:2454:ARG:NH2	1:B:2513:ASP:HB3	2.21	0.56
1:C:712:LEU:HD21	1:C:768:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:PHE:HA	1:D:281:TRP:CZ3	2.41	0.56
1:E:842:ALA:HB2	1:E:852:VAL:HG21	1.87	0.56
1:E:1246:TYR:HB3	1:E:1262:VAL:HG22	1.87	0.56
1:E:2453:ILE:HG13	1:E:2521:LEU:HD21	1.88	0.56
1:A:1046:PRO:HG2	1:A:1889:ARG:HH11	1.71	0.56
1:A:1846:ALA:HB1	1:A:1848:TRP:CE2	2.40	0.56
1:A:2484:PHE:CZ	1:E:2361:GLU:HB3	2.41	0.56
1:B:1439:ILE:HG13	1:B:1486:ASN:CB	2.36	0.56
1:C:1162:PHE:CD2	1:C:1241:LEU:HD21	2.41	0.56
1:D:732:PRO:HD2	1:D:760:PHE:CE2	2.41	0.56
1:D:784:LEU:HB3	1:D:789:PHE:CE2	2.40	0.56
1:B:129:LEU:HD21	1:B:1018:PHE:HZ	1.71	0.56
1:B:326:LYS:HB3	1:B:328:GLU:OE1	2.06	0.56
1:C:742:THR:O	1:C:746:LYS:HD3	2.05	0.56
1:C:1227:ARG:HH12	1:C:1229:ALA:HB2	1.69	0.56
1:D:349:LEU:HA	1:D:359:ILE:H	1.70	0.56
1:D:1821:LYS:NZ	1:D:1896:LEU:HD12	2.20	0.56
1:E:1415:TYR:CE2	1:E:1468:VAL:HG21	2.41	0.56
1:A:2002:ARG:HE	1:B:977:VAL:HG12	1.70	0.55
1:A:2229:ASN:HD21	1:E:2126:ARG:HD3	1.72	0.55
1:A:2299:LEU:HD22	1:E:2350:LYS:HD3	1.87	0.55
1:B:324:GLU:HB2	1:B:351:TYR:HB2	1.88	0.55
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.88	0.55
1:B:1416:ASN:O	1:B:1420:ASN:CA	2.53	0.55
1:C:760:PHE:CE2	1:C:764:MET:HE3	2.42	0.55
1:D:1162:PHE:CD2	1:D:1163:ARG:HG2	2.41	0.55
1:D:1889:ARG:O	1:D:1892:ASP:HB2	2.06	0.55
1:E:420:TYR:CZ	1:E:426:ALA:HB2	2.41	0.55
1:E:1226:GLU:HB3	1:E:1247:LYS:HG3	1.87	0.55
1:E:1664:LEU:HB2	1:E:1705:THR:OG1	2.06	0.55
1:A:816:TRP:O	1:A:820:LEU:HG	2.07	0.55
1:A:1174:GLU:HB2	1:A:1189:ARG:HG2	1.88	0.55
1:B:1137:ALA:HB3	1:B:1861:TRP:HE3	1.71	0.55
1:B:2126:ARG:HD3	1:C:2229:ASN:HD21	1.71	0.55
1:C:1371:ARG:HG3	1:C:1372:ASN:N	2.21	0.55
1:D:465:LEU:HA	1:D:468:ILE:HG22	1.88	0.55
1:D:554:THR:HG22	1:D:556:ALA:H	1.71	0.55
1:A:26:GLN:CG	1:A:27:TYR:HA	2.36	0.55
1:A:328:GLU:HG2	1:A:438:SER:HB2	1.88	0.55
1:A:2459:TYR:CZ	1:A:2461:GLY:HA3	2.41	0.55
1:B:350:MET:HE1	1:B:359:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLU:HA	1:C:259:ALA:HB2	1.88	0.55
1:D:202:PRO:O	1:D:206:ILE:HG12	2.06	0.55
1:D:358:PHE:HE1	1:D:414:LYS:O	1.90	0.55
1:D:406:ASP:HA	1:D:409:TYR:HB2	1.89	0.55
1:D:1169:ILE:HD11	1:D:1192:LEU:HG	1.88	0.55
1:E:1413:THR:HA	1:E:1424:SER:HA	1.89	0.55
1:A:2308:GLN:NE2	1:A:2321:THR:HA	2.21	0.55
1:B:129:LEU:HD13	1:B:1012:VAL:HG13	1.88	0.55
1:B:410:LYS:HA	1:B:436:PHE:O	2.07	0.55
1:B:1313:PHE:HE2	1:B:1345:TYR:CE1	2.25	0.55
1:C:1810:PRO:HA	1:C:1829:TRP:HE1	1.70	0.55
1:D:684:ARG:HD3	1:D:744:VAL:O	2.07	0.55
1:E:1125:VAL:HB	1:E:1140:TRP:CE3	2.41	0.55
1:E:2242:GLU:HA	1:E:2245:LYS:NZ	2.21	0.55
1:A:1287:LEU:HD11	1:A:1309:PHE:HB2	1.87	0.55
1:A:1885:ALA:O	1:A:1889:ARG:HG2	2.06	0.55
1:B:545:SER:HB2	1:B:586:THR:HG22	1.88	0.55
1:B:1415:TYR:CE1	1:B:1473:THR:HG22	2.42	0.55
1:B:1626:LEU:HD23	1:B:1626:LEU:H	1.71	0.55
1:C:1314:GLU:HB3	1:C:1591:LYS:HB2	1.88	0.55
1:C:2273:GLN:NE2	1:C:2274:ARG:HG2	2.22	0.55
1:C:2439:VAL:HG22	1:C:2532:ILE:HD12	1.88	0.55
1:C:2472:ILE:HD11	1:C:2495:PRO:HB2	1.86	0.55
1:D:355:ASN:HD21	1:D:400:TYR:HB2	1.70	0.55
1:D:964:ARG:HB3	1:D:976:GLN:NE2	2.20	0.55
1:E:1162:PHE:CD1	1:E:1241:LEU:HD21	2.41	0.55
1:E:1230:LEU:HA	1:E:1244:PHE:O	2.06	0.55
1:A:532:LEU:N	1:A:562:ARG:HH22	2.04	0.55
1:A:582:ASP:HB3	1:A:586:THR:OG1	2.06	0.55
1:A:1319:LEU:HD11	1:A:1588:LEU:HD13	1.89	0.55
1:A:2335:LEU:C	1:A:2336:MET:HG3	2.32	0.55
1:B:1610:ALA:HB2	1:B:1652:PRO:HG2	1.88	0.55
1:C:1839:TYR:CE1	1:C:1851:ASN:HB2	2.41	0.55
1:E:276:PHE:HD2	1:E:281:TRP:HZ3	1.55	0.55
1:E:897:ARG:H	1:E:908:ASN:HB3	1.71	0.55
1:A:1714:ALA:HB3	1:A:1717:TYR:HB2	1.89	0.55
1:A:1997:ARG:HH11	1:A:2007:ILE:HD11	1.70	0.55
1:A:2264:HIS:CE1	1:E:2090:GLN:HB3	2.42	0.55
1:A:2336:MET:HE1	1:B:2288:LYS:HB2	1.87	0.55
1:B:77:GLY:N	1:B:1925:GLY:HA3	2.19	0.55
1:B:719:MET:HE3	1:B:778:GLU:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1362:ARG:HE	1:B:1363:TYR:N	2.04	0.55
1:C:184:LEU:O	1:C:188:LEU:HG	2.07	0.55
1:C:219:ALA:HA	1:C:222:ARG:HE	1.71	0.55
1:C:1246:TYR:HB3	1:C:1262:VAL:HG22	1.88	0.55
1:C:1662:PHE:HZ	1:C:1725:LEU:HD13	1.72	0.55
1:C:2129:LYS:HG2	1:D:2225:ILE:HG22	1.88	0.55
1:D:11:ILE:HD11	1:D:41:LEU:HD23	1.88	0.55
1:D:551:GLU:HG3	1:D:552:GLN:HG2	1.89	0.55
1:D:901:ALA:N	1:D:907:SER:HB2	2.17	0.55
1:D:2116:LEU:HD22	1:D:2244:LEU:HD12	1.87	0.55
1:E:1400:LYS:HD3	1:E:1401:HIS:O	2.07	0.55
1:E:2056:ARG:HA	1:E:2059:ASN:HD21	1.71	0.55
1:E:2088:LEU:HB3	1:E:2269:LEU:HD12	1.89	0.55
1:A:226:VAL:HG21	1:A:879:VAL:HG21	1.89	0.55
1:A:1342:THR:HG22	1:A:1355:HIS:HE1	1.71	0.55
1:B:296:TYR:CZ	1:B:462:PRO:HG3	2.42	0.55
1:B:434:PHE:CZ	1:B:436:PHE:HB2	2.42	0.55
1:B:2090:GLN:HE22	1:C:2268:GLN:HB2	1.72	0.55
1:C:854:GLN:CD	1:C:886:MET:HE2	2.32	0.55
1:C:2267:ALA:HA	1:C:2270:GLU:OE1	2.07	0.55
1:C:2359:ALA:HB1	1:C:2535:THR:HB	1.88	0.55
1:D:2324:ARG:NH1	1:D:2324:ARG:HB2	2.22	0.55
1:E:1123:ARG:HD2	1:E:1143:TRP:CH2	2.42	0.55
1:E:1447:TYR:CD2	1:E:1490:GLY:HA2	2.42	0.55
1:A:420:TYR:CZ	1:A:426:ALA:HB2	2.42	0.55
1:A:793:GLY:HA3	1:A:868:GLN:HG2	1.87	0.55
1:A:1082:THR:O	1:A:1085:GLU:HG3	2.07	0.55
1:B:1422:ILE:HB	1:B:1466:PHE:HB2	1.89	0.55
1:B:2120:ARG:HA	1:B:2237:MET:HE3	1.88	0.55
1:B:2198:LEU:HA	1:B:2201:THR:HG22	1.88	0.55
1:C:346:TYR:OH	1:C:364:LYS:HG3	2.06	0.55
1:D:129:LEU:HD13	1:D:1012:VAL:HG13	1.89	0.55
1:D:276:PHE:HD1	1:D:281:TRP:HZ3	1.55	0.55
1:D:1371:ARG:HG3	1:D:1372:ASN:N	2.22	0.55
1:E:27:TYR:HB3	1:E:28:LEU:HD22	1.87	0.55
1:E:236:LEU:HD13	1:E:487:PHE:HB2	1.89	0.55
1:E:297:LEU:HD23	1:E:297:LEU:H	1.72	0.55
1:E:1227:ARG:HH12	1:E:1229:ALA:HB2	1.71	0.55
1:A:1413:THR:HA	1:A:1423:ALA:O	2.07	0.55
1:B:2191:ALA:O	1:B:2195:VAL:HG13	2.07	0.55
1:C:1211:ILE:HG22	1:C:1265:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1839:TYR:CZ	1:C:1851:ASN:HB2	2.42	0.55
1:D:27:TYR:HB3	1:D:28:LEU:HD22	1.87	0.55
1:D:1123:ARG:HD2	1:D:1143:TRP:CH2	2.42	0.55
1:E:360:ARG:HB2	1:E:365:VAL:HG22	1.88	0.55
1:E:1150:VAL:HG23	1:E:1170:TRP:CE2	2.42	0.55
1:A:1288:LYS:HA	1:A:1291:PHE:CE1	2.41	0.54
1:B:1049:ARG:O	1:B:1052:GLN:HG3	2.08	0.54
1:D:219:ALA:HA	1:D:222:ARG:HE	1.72	0.54
1:D:1920:THR:HG23	1:D:1994:LEU:HD21	1.89	0.54
1:E:1489:GLN:HE22	1:E:1491:PHE:N	2.05	0.54
1:E:1519:MET:HB2	1:E:1568:ASP:OD1	2.07	0.54
1:E:2500:SER:HB3	1:E:2503:ASP:HB2	1.88	0.54
1:B:236:LEU:HD13	1:B:487:PHE:HB2	1.89	0.54
1:B:527:PHE:CD1	1:B:563:GLY:HA3	2.42	0.54
1:B:1092:VAL:HG21	1:B:1109:PHE:HB3	1.89	0.54
1:B:1123:ARG:HD2	1:B:1143:TRP:CH2	2.42	0.54
1:C:76:SER:HB3	1:C:80:ARG:HE	1.72	0.54
1:D:404:ILE:HG13	1:D:414:LYS:HD3	1.87	0.54
1:D:777:SER:HB3	1:D:2274:ARG:HH12	1.72	0.54
1:A:439:TYR:HB3	1:A:440:PRO:O	2.07	0.54
1:A:1170:TRP:CE2	1:A:1193:LYS:HB2	2.42	0.54
1:A:1350:LEU:HB3	1:A:1555:ALA:O	2.07	0.54
1:A:1508:GLY:C	1:A:1576:LYS:HE3	2.32	0.54
1:A:1570:VAL:HA	1:A:1584:ILE:O	2.07	0.54
1:B:1804:GLU:HA	1:B:1808:TYR:HB2	1.89	0.54
1:B:2104:ARG:HD2	1:C:2246:ILE:HD11	1.89	0.54
1:C:489:THR:HA	1:C:503:ALA:HB1	1.90	0.54
1:C:1821:LYS:NZ	1:C:1896:LEU:HD12	2.22	0.54
1:C:2367:SER:HB2	1:D:2450:TYR:CD1	2.43	0.54
1:D:29:SER:HB2	1:D:1015:ARG:HA	1.88	0.54
1:D:919:ALA:O	1:D:923:GLU:HG3	2.07	0.54
1:E:760:PHE:HA	1:E:763:VAL:HG12	1.89	0.54
1:E:1350:LEU:HB3	1:E:1555:ALA:O	2.07	0.54
1:E:1642:LEU:HD12	1:E:1832:TYR:CD1	2.42	0.54
1:A:29:SER:HB2	1:A:1015:ARG:HA	1.88	0.54
1:C:1130:MET:HE3	1:C:1133:GLY:H	1.72	0.54
1:C:1885:ALA:O	1:C:1889:ARG:HG2	2.07	0.54
1:C:2308:GLN:NE2	1:C:2321:THR:HA	2.23	0.54
1:E:76:SER:HB3	1:E:80:ARG:HE	1.72	0.54
1:A:1037:VAL:HG13	1:A:1038:TYR:CD1	2.43	0.54
1:A:1163:ARG:O	1:A:1164:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1672:HIS:HD2	1:A:1729:TYR:CD2	2.26	0.54
1:A:2184:ARG:NH2	1:E:2184:ARG:HH22	2.05	0.54
1:B:1162:PHE:CD1	1:B:1241:LEU:HD21	2.43	0.54
1:C:2064:LEU:HD11	1:C:2300:THR:HG21	1.88	0.54
1:D:2350:LYS:HB2	1:E:2299:LEU:HD11	1.88	0.54
1:E:336:LYS:HG2	1:E:339:ASP:CB	2.31	0.54
1:E:1096:TYR:HD1	1:E:1306:SER:HB2	1.72	0.54
1:A:2242:GLU:HA	1:A:2245:LYS:HZ2	1.73	0.54
1:B:346:TYR:HE2	1:B:365:VAL:HA	1.73	0.54
1:B:351:TYR:HB3	1:B:356:GLN:HE22	1.71	0.54
1:B:727:THR:HG21	1:B:764:MET:SD	2.47	0.54
1:C:1243:VAL:HG23	1:C:1265:MET:HB3	1.89	0.54
1:C:1405:TYR:HB2	1:C:1430:MET:HE1	1.90	0.54
1:C:1629:GLN:HG2	1:C:1649:LEU:HD11	1.88	0.54
1:C:2028:THR:HG21	1:D:2270:GLU:HB2	1.89	0.54
1:D:1287:LEU:HD21	1:D:1309:PHE:HB2	1.89	0.54
1:D:1967:LYS:HG3	1:D:1968:ASN:H	1.71	0.54
1:E:1722:GLY:H	1:E:1766:GLN:CG	2.19	0.54
1:A:286:TYR:HB3	1:A:288:LEU:HD13	1.88	0.54
1:A:897:ARG:H	1:A:908:ASN:HB3	1.72	0.54
1:A:2132:GLN:O	1:A:2136:GLU:HG3	2.07	0.54
1:A:2184:ARG:HD3	1:A:2190:ARG:HH22	1.72	0.54
1:B:743:LEU:HD11	1:B:757:LEU:HD13	1.89	0.54
1:B:2164:ILE:HG21	1:E:1119:GLU:OE2	2.07	0.54
1:B:2339:GLU:HG3	1:C:2067:PHE:HE1	1.71	0.54
1:C:887:PRO:HA	1:C:890:ILE:HG12	1.89	0.54
1:D:1629:GLN:O	1:D:1633:ARG:HG2	2.08	0.54
1:D:2056:ARG:HA	1:D:2059:ASN:HD21	1.73	0.54
1:D:2261:GLN:HA	1:D:2264:HIS:CE1	2.43	0.54
1:E:126:ALA:HA	1:E:129:LEU:HD23	1.90	0.54
1:E:2261:GLN:HA	1:E:2264:HIS:CE1	2.43	0.54
1:A:76:SER:HB2	1:A:80:ARG:HH21	1.72	0.54
1:A:2472:ILE:HD11	1:A:2495:PRO:HB2	1.90	0.54
1:B:370:GLY:H	1:B:386:LEU:HB2	1.73	0.54
1:C:1169:ILE:HD11	1:C:1192:LEU:HG	1.90	0.54
1:C:1350:LEU:HB3	1:C:1555:ALA:O	2.08	0.54
1:C:2104:ARG:HD2	1:D:2246:ILE:HD11	1.88	0.54
1:D:95:MET:HE1	1:D:1971:THR:HB	1.90	0.54
1:D:1534:ALA:HB2	1:D:1548:PHE:C	2.33	0.54
1:D:1675:GLU:HB3	1:D:1677:TRP:CD1	2.43	0.54
1:E:732:PRO:HD2	1:E:760:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1324:ALA:HB3	1:E:1584:ILE:HD11	1.89	0.54
1:A:298:GLY:H	1:A:315:ILE:HA	1.72	0.54
1:A:576:LYS:HG2	1:A:581:LEU:HD11	1.89	0.54
1:A:2102:GLN:HB3	1:A:2254:GLN:HE22	1.72	0.54
1:A:2242:GLU:HA	1:A:2245:LYS:NZ	2.23	0.54
1:B:600:LEU:HD23	1:B:603:LEU:HD12	1.89	0.54
1:C:126:ALA:HA	1:C:129:LEU:HD23	1.90	0.54
1:C:719:MET:HE3	1:C:778:GLU:OE1	2.08	0.54
1:D:192:ARG:HE	1:D:249:ILE:HD11	1.73	0.54
1:D:1230:LEU:HA	1:D:1244:PHE:O	2.08	0.54
1:E:176:LYS:HD3	1:E:954:ILE:HG13	1.90	0.54
1:E:2045:LEU:HD23	1:E:2466:PRO:HD2	1.89	0.54
1:A:184:LEU:O	1:A:188:LEU:HG	2.07	0.54
1:A:346:TYR:HA	1:A:361:ALA:HB3	1.90	0.54
1:A:1477:LYS:NZ	1:A:1502:TRP:HB2	2.22	0.54
1:A:2297:PHE:CE2	1:A:2328:TRP:HB2	2.43	0.54
1:B:680:LEU:HD13	1:B:744:VAL:HG13	1.90	0.54
1:C:357:PHE:CZ	1:C:397:LYS:HG2	2.43	0.54
1:C:2363:THR:OG1	1:C:2533:ARG:HG2	2.08	0.54
1:D:577:LEU:HD11	1:D:615:CYS:SG	2.48	0.54
1:D:2109:VAL:O	1:D:2113:ILE:HG12	2.08	0.54
1:D:2335:LEU:C	1:D:2336:MET:HG3	2.33	0.54
1:D:2336:MET:HB2	1:D:2339:GLU:OE2	2.08	0.54
1:E:172:HIS:HA	1:E:175:ARG:NH1	2.23	0.54
1:E:784:LEU:HB3	1:E:789:PHE:CE1	2.43	0.54
1:A:321:VAL:HG12	1:A:351:TYR:CD2	2.43	0.53
1:A:1158:ARG:HH11	1:A:1231:ALA:HA	1.72	0.53
1:A:1967:LYS:HG3	1:A:1968:ASN:H	1.73	0.53
1:B:1037:VAL:HG13	1:B:1038:TYR:CD1	2.43	0.53
1:B:2308:GLN:NE2	1:B:2321:THR:HA	2.23	0.53
1:C:14:THR:HB	1:C:20:MET:HB3	1.90	0.53
1:C:217:LEU:HB3	1:C:220:LEU:HB3	1.88	0.53
1:C:582:ASP:HB3	1:C:586:THR:OG1	2.08	0.53
1:C:739:GLY:HA2	1:C:742:THR:HG22	1.90	0.53
1:C:1084:PHE:HE2	1:C:1801:TYR:HB3	1.73	0.53
1:D:360:ARG:CG	1:D:398:SER:HB2	2.38	0.53
1:E:582:ASP:HB3	1:E:586:THR:OG1	2.07	0.53
1:A:192:ARG:HG2	1:A:266:ASN:HA	1.90	0.53
1:C:789:PHE:HB2	1:C:799:ALA:HA	1.90	0.53
1:C:1153:TYR:CD1	1:C:1173:LYS:HE3	2.43	0.53
1:D:33:LEU:HA	1:D:36:ILE:HG12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ASP:O	1:D:504:GLN:HG2	2.08	0.53
1:E:126:ALA:HB2	1:E:997:ILE:HD11	1.89	0.53
1:E:1378:MET:HE1	1:E:1393:PHE:CD2	2.43	0.53
1:A:2053:MET:HA	1:A:2056:ARG:HG2	1.90	0.53
1:B:339:ASP:OD2	1:B:343:ASN:HB2	2.08	0.53
1:B:350:MET:HG2	1:B:395:ASN:ND2	2.24	0.53
1:B:576:LYS:HG2	1:B:581:LEU:HD11	1.90	0.53
1:B:2028:THR:HG21	1:C:2270:GLU:HB2	1.91	0.53
1:D:2071:LEU:HA	1:D:2074:MET:HE3	1.90	0.53
1:E:820:LEU:HB3	1:E:824:GLY:HA3	1.88	0.53
1:A:297:LEU:HD23	1:A:297:LEU:H	1.73	0.53
1:B:67:ILE:HD11	1:B:89:SER:HA	1.89	0.53
1:B:126:ALA:HA	1:B:129:LEU:HD23	1.90	0.53
1:B:1571:PHE:HB2	1:B:1584:ILE:HB	1.91	0.53
1:B:1574:LYS:HA	1:B:1581:LEU:H	1.74	0.53
1:C:72:ASN:HB3	1:C:75:LEU:HD13	1.91	0.53
1:C:684:ARG:HG2	1:C:745:LEU:HA	1.90	0.53
1:C:702:GLU:HG2	1:C:721:ARG:HD2	1.90	0.53
1:C:1021:TRP:CH2	1:C:1025:ASN:HA	2.44	0.53
1:C:2160:GLN:HG3	1:C:2198:LEU:HD11	1.90	0.53
1:E:310:ALA:HB3	1:E:330:TYR:CE2	2.44	0.53
1:E:349:LEU:HD11	1:E:404:ILE:HG22	1.90	0.53
1:E:2242:GLU:HA	1:E:2245:LYS:HZ2	1.73	0.53
1:E:2308:GLN:HE22	1:E:2321:THR:HG23	1.74	0.53
1:B:1413:THR:HA	1:B:1424:SER:HA	1.91	0.53
1:C:1108:TRP:CE2	1:C:1161:ILE:HD11	2.44	0.53
1:D:527:PHE:CD1	1:D:563:GLY:HA3	2.44	0.53
1:D:2184:ARG:HG2	1:D:2187:ALA:HB2	1.90	0.53
1:E:26:GLN:CG	1:E:27:TYR:HA	2.38	0.53
1:E:206:ILE:HD11	1:E:919:ALA:HA	1.90	0.53
1:E:336:LYS:HA	1:E:432:GLY:HA3	1.89	0.53
1:E:816:TRP:CE2	1:E:820:LEU:HD21	2.43	0.53
1:E:1544:MET:HB3	1:E:1546:TYR:HE2	1.73	0.53
1:E:2075:ALA:HA	1:E:2286:ARG:NH2	2.23	0.53
1:A:532:LEU:HD11	1:E:923:GLU:HG2	1.90	0.53
1:A:1666:LYS:HE2	1:A:1703:SER:HA	1.91	0.53
1:A:2164:ILE:HG22	1:D:1117:LEU:HD12	1.90	0.53
1:B:272:THR:HG22	1:B:275:ASN:OD1	2.08	0.53
1:B:1106:LEU:HB3	1:B:1108:TRP:HE1	1.73	0.53
1:C:350:MET:CG	1:C:359:ILE:HG13	2.38	0.53
1:C:1130:MET:SD	1:C:1135:LEU:HD23	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1399:VAL:HA	1:E:1498:GLN:O	2.08	0.53
1:E:1934:GLN:H	1:E:1934:GLN:CD	2.17	0.53
1:E:2095:ALA:O	1:E:2099:ILE:HG12	2.08	0.53
1:A:548:PRO:HB2	1:E:886:MET:HE1	1.91	0.53
1:A:1304:LYS:HG2	1:A:1602:PHE:HB3	1.91	0.53
1:A:2308:GLN:HA	1:A:2348:MET:HE1	1.91	0.53
1:A:2511:PHE:HD2	1:A:2522:LEU:HD12	1.73	0.53
1:B:373:LEU:HD23	1:B:381:GLY:H	1.73	0.53
1:C:310:ALA:HB3	1:C:330:TYR:CE2	2.44	0.53
1:C:1437:ARG:O	1:C:1439:ILE:HG12	2.09	0.53
1:C:1959:MET:HA	1:C:1962:ARG:NH2	2.24	0.53
1:D:1413:THR:HA	1:D:1424:SER:HA	1.90	0.53
1:E:347:PHE:O	1:E:415:ILE:HD13	2.09	0.53
1:E:801:GLN:O	1:E:806:THR:HG21	2.09	0.53
1:E:1338:ILE:HG13	1:E:1338:ILE:O	2.09	0.53
1:E:2192:SER:O	1:E:2195:VAL:HG22	2.08	0.53
1:A:470:ARG:HD2	1:A:514:TYR:CE2	2.42	0.53
1:A:852:VAL:O	1:A:856:MET:HG2	2.09	0.53
1:B:642:TRP:O	1:B:645:GLN:HG2	2.09	0.53
1:B:1363:TYR:HE2	1:B:1389:TYR:HE1	1.57	0.53
1:D:333:THR:H	1:D:435:THR:HB	1.74	0.53
1:D:1489:GLN:HG3	1:D:1492:GLN:HB2	1.89	0.53
1:D:1555:ALA:HB1	1:D:1558:LEU:HD21	1.91	0.53
1:D:1676:ARG:NH2	1:D:1698:MET:HE3	2.24	0.53
1:E:1265:MET:HE2	1:E:1265:MET:HA	1.91	0.53
1:E:1431:ASN:HD22	1:E:1494:PHE:HZ	1.57	0.53
1:E:1932:GLY:HA2	1:E:1935:GLN:HE21	1.73	0.53
1:A:527:PHE:CZ	1:A:594:ILE:HD11	2.43	0.53
1:B:350:MET:CE	1:B:359:ILE:HG13	2.39	0.53
1:B:613:GLU:HG3	1:B:657:THR:OG1	2.09	0.53
1:D:48:HIS:O	1:D:52:GLU:HG2	2.09	0.53
1:D:657:THR:O	1:D:660:ILE:HG22	2.08	0.53
1:D:784:LEU:HB3	1:D:789:PHE:HE2	1.72	0.53
1:D:977:VAL:HB	1:D:981:ILE:HD13	1.90	0.53
1:D:1333:MET:HE1	1:D:1582:GLY:HA3	1.90	0.53
1:D:1539:ASN:HA	1:D:1544:MET:HE1	1.91	0.53
1:E:199:TYR:CD1	1:E:945:VAL:HG21	2.44	0.53
1:A:32:GLU:HB3	1:A:1011:ASP:HB2	1.91	0.53
1:A:117:GLY:HA2	1:A:120:THR:HG22	1.91	0.53
1:A:623:PHE:HD2	1:A:639:LEU:HD13	1.74	0.53
1:A:2261:GLN:HA	1:A:2264:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:ARG:O	1:C:603:LEU:HG	2.08	0.53
1:D:223:ASN:O	1:D:226:VAL:HG22	2.09	0.53
1:D:545:SER:HA	1:D:586:THR:HA	1.90	0.53
1:D:2164:ILE:HG12	1:D:2195:VAL:HG11	1.90	0.53
1:E:349:LEU:HD21	1:E:404:ILE:HB	1.91	0.53
1:A:2292:ILE:HD13	1:E:2339:GLU:HG2	1.91	0.52
1:B:353:GLY:H	1:B:357:PHE:HZ	1.55	0.52
1:B:901:ALA:N	1:B:907:SER:HB2	2.20	0.52
1:B:1316:PRO:HD2	1:B:1588:LEU:HD11	1.91	0.52
1:D:347:PHE:HB3	1:D:415:ILE:HG23	1.90	0.52
1:D:789:PHE:HB2	1:D:799:ALA:HA	1.90	0.52
1:D:1436:ARG:HA	1:D:1487:ASN:HD21	1.75	0.52
1:D:2360:LEU:HD11	1:E:2472:ILE:HD12	1.92	0.52
1:E:513:GLN:HG3	1:E:514:TYR:HD1	1.73	0.52
1:E:722:TYR:HB3	1:E:785:VAL:HG11	1.91	0.52
1:A:1839:TYR:CE1	1:A:1851:ASN:HB2	2.45	0.52
1:A:2118:GLU:OE2	1:B:2236:GLN:HA	2.09	0.52
1:B:969:SER:O	1:B:972:LEU:HD22	2.09	0.52
1:B:1487:ASN:N	1:B:1489:GLN:HE22	2.01	0.52
1:B:1523:LYS:HZ2	1:B:1557:SER:HB2	1.74	0.52
1:C:236:LEU:HA	1:C:487:PHE:CD1	2.45	0.52
1:C:336:LYS:HB2	1:C:431:GLY:C	2.33	0.52
1:C:578:ALA:HA	1:C:628:THR:HG22	1.91	0.52
1:D:2206:SER:O	1:D:2209:LYS:HG3	2.10	0.52
1:D:2372:TYR:HD2	1:D:2382:LEU:HD13	1.74	0.52
1:E:1056:MET:HE3	1:E:1812:MET:HE3	1.91	0.52
1:E:1082:THR:O	1:E:1085:GLU:HG3	2.09	0.52
1:A:336:LYS:NZ	1:A:430:GLY:HA3	2.24	0.52
1:A:1169:ILE:HD11	1:A:1192:LEU:HG	1.92	0.52
1:B:167:GLU:O	1:B:171:GLU:HG2	2.10	0.52
1:B:602:LEU:HD23	1:B:605:ARG:HD3	1.92	0.52
1:B:2050:PHE:HE2	1:B:2311:LEU:HB2	1.74	0.52
1:B:2297:PHE:HA	1:B:2300:THR:HG22	1.90	0.52
1:C:297:LEU:HD12	1:C:316:SER:HB2	1.91	0.52
1:C:437:GLU:HB2	1:C:439:TYR:CE1	2.44	0.52
1:D:856:MET:SD	1:D:861:VAL:HG23	2.49	0.52
1:D:1472:LYS:HB3	1:D:1475:ASP:HB3	1.91	0.52
1:D:2358:ARG:HB2	1:E:2047:LEU:HD21	1.89	0.52
1:E:1338:ILE:HG13	1:E:1341:ILE:HD11	1.91	0.52
1:E:2393:GLY:O	1:E:2406:LEU:HD22	2.10	0.52
1:A:642:TRP:O	1:A:645:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:GLN:O	1:A:2066:GLN:HG3	2.09	0.52
1:B:1998:LEU:O	1:B:2002:ARG:HG2	2.09	0.52
1:B:2459:TYR:CZ	1:B:2461:GLY:HA3	2.45	0.52
1:C:324:GLU:HB3	1:C:351:TYR:CD2	2.45	0.52
1:C:1431:ASN:ND2	1:C:1434:TYR:HB2	2.25	0.52
1:D:27:TYR:HD2	1:D:28:LEU:HD22	1.74	0.52
1:A:2437:LYS:HZ1	1:B:2484:PHE:HE2	1.58	0.52
1:B:375:LYS:HG3	1:B:413:VAL:HG21	1.91	0.52
1:B:1021:TRP:CH2	1:B:1025:ASN:HA	2.45	0.52
1:B:2328:TRP:CD2	1:B:2334:GLY:HA3	2.44	0.52
1:C:239:LEU:HB3	1:C:487:PHE:HE1	1.75	0.52
1:D:334:ARG:HD3	1:D:334:ARG:H	1.75	0.52
1:D:1846:ALA:HB1	1:D:1848:TRP:CE2	2.45	0.52
1:E:25:LEU:CA	1:E:27:TYR:HB2	2.39	0.52
1:E:168:LEU:O	1:E:171:GLU:HG3	2.08	0.52
1:E:290:LEU:HA	1:E:293:VAL:HG22	1.91	0.52
1:E:1436:ARG:HG3	1:E:1456:PHE:CE2	2.45	0.52
1:A:2053:MET:HE1	1:A:2306:MET:CB	2.40	0.52
1:B:551:GLU:HG3	1:B:552:GLN:HG2	1.91	0.52
1:B:2095:ALA:O	1:B:2099:ILE:HG12	2.10	0.52
1:D:334:ARG:HB2	1:D:434:PHE:HA	1.92	0.52
1:D:1084:PHE:HA	1:D:1087:VAL:HG12	1.92	0.52
1:D:1355:HIS:CD2	1:D:1550:PRO:HB3	2.45	0.52
1:D:1714:ALA:HB3	1:D:1717:TYR:HB2	1.91	0.52
1:E:191:TYR:CD2	1:E:197:THR:HG21	2.45	0.52
1:A:984:THR:HG23	1:A:987:ALA:H	1.74	0.52
1:A:1092:VAL:HG21	1:A:1109:PHE:HD2	1.75	0.52
1:A:1649:LEU:HD12	1:A:1650:PRO:HD2	1.92	0.52
1:B:297:LEU:HD23	1:B:297:LEU:H	1.75	0.52
1:B:774:LEU:HB3	1:B:776:LEU:HD23	1.91	0.52
1:B:1436:ARG:HB2	1:B:1485:GLY:HA2	1.90	0.52
1:B:1639:ASP:HA	1:B:1832:TYR:HE2	1.74	0.52
1:B:2048:TYR:HD2	1:B:2052:VAL:HG21	1.75	0.52
1:B:2063:GLN:O	1:B:2066:GLN:HG3	2.10	0.52
1:B:2284:TRP:HB3	1:B:2288:LYS:NZ	2.23	0.52
1:C:576:LYS:HG2	1:C:581:LEU:HD11	1.90	0.52
1:C:986:LEU:O	1:C:990:ILE:HG12	2.09	0.52
1:C:1234:GLY:O	1:C:1308:ARG:HG3	2.09	0.52
1:C:1422:ILE:HG23	1:C:1466:PHE:HB2	1.92	0.52
1:D:225:GLU:HB2	1:D:875:GLN:OE1	2.09	0.52
1:D:2350:LYS:HD3	1:E:2299:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ILE:HD11	1:E:395:ASN:OD1	2.09	0.52
1:E:620:LEU:HD13	1:E:664:CYS:HB3	1.91	0.52
1:A:755:THR:HA	1:A:758:VAL:HG22	1.92	0.52
1:A:1534:ALA:HB2	1:A:1548:PHE:C	2.35	0.52
1:A:2142:GLU:HB3	1:A:2216:TYR:HE2	1.75	0.52
1:B:2363:THR:OG1	1:B:2533:ARG:HG2	2.10	0.52
1:C:642:TRP:O	1:C:645:GLN:HG2	2.10	0.52
1:C:1371:ARG:HA	1:C:1375:ILE:HD13	1.92	0.52
1:C:2108:GLU:OE1	1:D:2246:ILE:HG23	2.10	0.52
1:D:15:ARG:N	1:D:15:ARG:HD3	2.24	0.52
1:D:310:ALA:HB3	1:D:330:TYR:CE2	2.44	0.52
1:D:1639:ASP:HA	1:D:1832:TYR:CE2	2.45	0.52
1:E:2438:GLN:HG2	1:E:2494:LEU:HD21	1.90	0.52
1:A:347:PHE:HD1	1:A:358:PHE:CZ	2.23	0.52
1:B:404:ILE:HG21	1:B:414:LYS:HG2	1.92	0.52
1:B:1123:ARG:HD2	1:B:1143:TRP:CZ2	2.45	0.52
1:C:409:TYR:O	1:C:436:PHE:HB3	2.10	0.52
1:C:1074:GLU:O	1:C:1078:LYS:HG2	2.09	0.52
1:D:2533:ARG:HD3	1:E:2484:PHE:CE1	2.45	0.52
1:E:1130:MET:HE2	1:E:1135:LEU:HD23	1.91	0.52
1:A:1021:TRP:CH2	1:A:1025:ASN:HA	2.44	0.52
1:A:1638:ILE:H	1:A:1638:ILE:HD12	1.75	0.52
1:B:491:PHE:CZ	1:B:495:ARG:HD3	2.45	0.52
1:B:900:THR:HG22	1:B:909:LEU:HD11	1.92	0.52
1:B:1135:LEU:HD11	1:B:1140:TRP:HE1	1.74	0.52
1:C:1644:MET:O	1:C:1648:ARG:HG2	2.09	0.52
1:D:162:LEU:HD21	1:D:977:VAL:O	2.10	0.52
1:D:414:LYS:O	1:D:415:ILE:HD13	2.10	0.52
1:E:249:ILE:HG22	1:E:453:ARG:NH2	2.24	0.52
1:E:854:GLN:OE1	1:E:886:MET:HG2	2.10	0.52
1:E:1639:ASP:HA	1:E:1832:TYR:CE1	2.45	0.52
1:A:578:ALA:HA	1:A:628:THR:HG22	1.91	0.51
1:C:346:TYR:HD1	1:C:361:ALA:HB3	1.74	0.51
1:C:602:LEU:HD23	1:C:605:ARG:HD3	1.91	0.51
1:E:33:LEU:HD13	1:E:50:TYR:HD1	1.75	0.51
1:E:330:TYR:O	1:E:331:LYS:HE2	2.09	0.51
1:E:2381:ASN:HB3	1:E:2384:GLU:HB3	1.93	0.51
1:A:346:TYR:CE1	1:A:360:ARG:HA	2.38	0.51
1:A:1436:ARG:HG3	1:A:1456:PHE:CE2	2.44	0.51
1:A:1629:GLN:O	1:A:1633:ARG:HG2	2.10	0.51
1:A:2050:PHE:CE2	1:A:2054:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2053:MET:HA	1:B:2056:ARG:HG2	1.91	0.51
1:C:26:GLN:HB3	1:C:27:TYR:HA	1.90	0.51
1:C:1644:MET:HG3	1:C:1848:TRP:CE2	2.45	0.51
1:C:1662:PHE:HB2	1:C:1707:MET:SD	2.49	0.51
1:D:236:LEU:HA	1:D:487:PHE:CD1	2.45	0.51
1:D:768:SER:O	1:D:772:GLN:HG2	2.10	0.51
1:D:2363:THR:OG1	1:D:2533:ARG:HG2	2.10	0.51
1:E:28:LEU:HD12	1:E:32:GLU:HG3	1.91	0.51
1:B:216:THR:HG22	1:B:494:HIS:HB3	1.93	0.51
1:B:1831:ASN:HA	1:B:1834:TYR:O	2.10	0.51
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.91	0.51
1:D:217:LEU:HB3	1:D:220:LEU:HB3	1.91	0.51
1:D:620:LEU:HD13	1:D:664:CYS:HB3	1.91	0.51
1:D:1227:ARG:HH12	1:D:1229:ALA:HB2	1.75	0.51
1:E:357:PHE:CG	1:E:397:LYS:HE2	2.45	0.51
1:A:761:CYS:HA	1:A:764:MET:CE	2.38	0.51
1:A:2115:VAL:HG22	1:B:2239:ALA:HB1	1.92	0.51
1:A:2439:VAL:HG22	1:A:2532:ILE:HG13	1.92	0.51
1:B:191:TYR:CD2	1:B:197:THR:HG21	2.46	0.51
1:B:2192:SER:O	1:B:2195:VAL:HG22	2.10	0.51
1:C:1627:ALA:O	1:C:1631:VAL:HG23	2.11	0.51
1:C:2045:LEU:HD13	1:C:2309:GLU:HG2	1.92	0.51
1:C:2156:SER:HA	1:D:2196:MET:HE1	1.92	0.51
1:D:1804:GLU:O	1:D:1809:THR:HG23	2.10	0.51
1:D:2050:PHE:CE2	1:D:2054:LEU:HD11	2.46	0.51
1:E:1811:MET:SD	1:E:1886:THR:HG22	2.51	0.51
1:E:1846:ALA:HB1	1:E:1848:TRP:CE2	2.45	0.51
1:A:833:GLN:CD	1:A:834:GLN:H	2.17	0.51
1:B:207:ARG:HH21	1:B:240:ALA:HA	1.75	0.51
1:B:349:LEU:HD11	1:B:404:ILE:HB	1.93	0.51
1:B:1125:VAL:HB	1:B:1140:TRP:CE3	2.45	0.51
1:B:2049:ARG:HG2	1:B:2493:TYR:CD1	2.46	0.51
1:C:70:ARG:HE	1:C:1880:MET:HG2	1.76	0.51
1:C:1374:GLN:O	1:C:1378:MET:HG2	2.11	0.51
1:C:2328:TRP:CD2	1:C:2334:GLY:HA3	2.46	0.51
1:D:348:ASP:H	1:D:359:ILE:HG22	1.76	0.51
1:D:663:LEU:HD22	1:D:770:SER:OG	2.11	0.51
1:D:969:SER:O	1:D:972:LEU:HD22	2.09	0.51
1:D:1375:ILE:O	1:D:1379:LYS:HG3	2.11	0.51
1:D:2109:VAL:HG23	1:D:2247:ARG:HH21	1.74	0.51
1:E:1629:GLN:HG2	1:E:1649:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1713:TYR:HD1	1:E:1718:TYR:CZ	2.28	0.51
1:E:1714:ALA:HB3	1:E:1717:TYR:HB2	1.93	0.51
1:E:1913:ALA:O	1:E:1917:TYR:HD2	1.93	0.51
1:A:162:LEU:HD21	1:A:977:VAL:O	2.11	0.51
1:A:1130:MET:HE3	1:A:1133:GLY:H	1.76	0.51
1:A:1523:LYS:HE3	1:A:1555:ALA:HA	1.93	0.51
1:B:249:ILE:HA	1:B:252:GLU:CD	2.36	0.51
1:B:1378:MET:HE1	1:B:1393:PHE:CD2	2.45	0.51
1:C:198:PRO:HD2	1:C:246:LEU:HG	1.92	0.51
1:C:209:VAL:HB	1:C:922:MET:HE1	1.93	0.51
1:C:768:SER:O	1:C:772:GLN:HG2	2.10	0.51
1:D:332:ILE:HD11	1:D:436:PHE:CD1	2.46	0.51
1:D:582:ASP:HB3	1:D:586:THR:OG1	2.11	0.51
1:D:1627:ALA:O	1:D:1631:VAL:HG23	2.10	0.51
1:D:2129:LYS:HG2	1:E:2225:ILE:HG22	1.93	0.51
1:E:856:MET:SD	1:E:861:VAL:HG23	2.51	0.51
1:E:1997:ARG:O	1:E:2001:LEU:HD23	2.09	0.51
1:E:2051:PRO:O	1:E:2054:LEU:HB3	2.10	0.51
1:A:1439:ILE:HG23	1:A:1450:ARG:CG	2.40	0.51
1:B:48:HIS:O	1:B:52:GLU:HG2	2.11	0.51
1:B:545:SER:HA	1:B:586:THR:HA	1.93	0.51
1:B:1108:TRP:CE2	1:B:1161:ILE:HD11	2.46	0.51
1:B:2472:ILE:HG13	1:B:2473:ALA:N	2.25	0.51
1:D:276:PHE:HA	1:D:281:TRP:CE3	2.46	0.51
1:D:367:ARG:HD3	1:D:390:LEU:HD21	1.91	0.51
1:E:276:PHE:HD1	1:E:441:LEU:HD21	1.73	0.51
1:E:2339:GLU:OE1	1:E:2339:GLU:N	2.43	0.51
1:E:2372:TYR:HA	1:E:2375:LEU:HG	1.92	0.51
1:A:11:ILE:HA	1:A:40:GLN:NE2	2.26	0.51
1:A:331:LYS:HB2	1:A:437:GLU:CD	2.36	0.51
1:A:355:ASN:ND2	1:A:402:SER:HB3	2.25	0.51
1:A:1831:ASN:HA	1:A:1834:TYR:O	2.11	0.51
1:B:328:GLU:HB2	1:B:438:SER:HB2	1.92	0.51
1:B:1400:LYS:HG3	1:B:1498:GLN:HE21	1.76	0.51
1:B:2056:ARG:HA	1:B:2059:ASN:ND2	2.25	0.51
1:B:2242:GLU:HA	1:B:2245:LYS:HG2	1.93	0.51
1:C:111:SER:HB2	1:C:1982:GLU:HB2	1.93	0.51
1:D:30:PHE:O	1:D:33:LEU:HG	2.11	0.51
1:D:326:LYS:HG2	1:D:328:GLU:HB3	1.93	0.51
1:D:1050:ILE:HG21	1:D:1870:ASP:OD1	2.11	0.51
1:D:1441:THR:HG23	1:D:1444:GLU:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2052:VAL:O	1:D:2055:GLU:HG2	2.11	0.51
1:D:2327:ALA:HB1	1:D:2337:ALA:HB1	1.93	0.51
1:E:700:GLN:HA	1:E:703:ILE:HG12	1.92	0.51
1:A:30:PHE:O	1:A:33:LEU:HG	2.11	0.51
1:A:316:SER:HA	1:A:331:LYS:NZ	2.26	0.51
1:A:373:LEU:HD23	1:A:380:SER:H	1.76	0.51
1:A:498:LEU:HD13	1:A:502:ASP:HB3	1.93	0.51
1:A:1351:ALA:HB1	1:A:1552:GLU:OE2	2.10	0.51
1:A:2178:LEU:HD12	1:E:2178:LEU:HD21	1.92	0.51
1:B:527:PHE:HD1	1:B:563:GLY:HA3	1.76	0.51
1:B:1116:ASN:HB2	1:C:1207:TRP:CD1	2.45	0.51
1:B:1434:TYR:HD2	1:B:1492:GLN:HE22	1.57	0.51
1:B:1523:LYS:HE3	1:B:1555:ALA:HA	1.93	0.51
1:B:1762:SER:HB2	1:B:1769:ILE:HD11	1.93	0.51
1:B:2184:ARG:HG3	1:B:2187:ALA:HB2	1.93	0.51
1:C:191:TYR:HB3	1:C:197:THR:OG1	2.10	0.51
1:C:1059:LEU:HD12	1:C:1080:TYR:CB	2.41	0.51
1:C:1680:ILE:HB	1:C:1695:TYR:HB3	1.93	0.51
1:C:1960:LEU:HD12	1:C:1964:GLY:HA2	1.92	0.51
1:C:2146:MET:HE1	1:C:2213:SER:HA	1.92	0.51
1:C:2400:SER:C	1:C:2416:ARG:HH21	2.19	0.51
1:D:308:THR:HG23	1:D:395:ASN:ND2	2.26	0.51
1:D:580:VAL:O	1:D:587:ILE:HD13	2.10	0.51
1:D:816:TRP:NE1	1:D:820:LEU:HD21	2.26	0.51
1:D:1415:TYR:CE1	1:D:1473:THR:HG22	2.45	0.51
1:E:200:HIS:HB3	1:E:203:TYR:HB3	1.92	0.51
1:E:1394:ILE:HG12	1:E:1417:LYS:HZ2	1.75	0.51
1:E:1456:PHE:CZ	1:E:1461:ILE:HD12	2.46	0.51
1:A:2178:LEU:H	1:A:2178:LEU:HD23	1.76	0.51
1:B:236:LEU:HD22	1:B:487:PHE:HB2	1.93	0.51
1:B:276:PHE:HD2	1:B:441:LEU:HD21	1.76	0.51
1:B:582:ASP:HB3	1:B:586:THR:OG1	2.11	0.51
1:B:848:ASP:HB3	1:B:851:MET:HG2	1.92	0.51
1:B:1839:TYR:CE1	1:B:1851:ASN:HB2	2.46	0.51
1:C:349:LEU:O	1:C:350:MET:HE2	2.10	0.51
1:C:886:MET:HE1	1:D:548:PRO:HB2	1.93	0.51
1:C:1439:ILE:HG13	1:C:1486:ASN:CB	2.41	0.51
1:D:620:LEU:HB2	1:D:804:ILE:HD11	1.91	0.51
1:D:2474:LEU:HD11	1:D:2477:GLY:HA2	1.92	0.51
1:E:1415:TYR:CE1	1:E:1417:LYS:HG2	2.46	0.51
1:A:1045:ASP:OD1	1:A:1047:THR:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1823:PHE:HB3	1:A:1897:ARG:NH2	2.26	0.50
1:A:2302:SER:O	1:A:2305:LEU:HG	2.11	0.50
1:B:1678:PHE:HD1	1:B:1699:LEU:HG	1.76	0.50
1:B:2157:LEU:O	1:B:2157:LEU:HD23	2.12	0.50
1:C:346:TYR:HE1	1:C:362:ASN:HB2	1.76	0.50
1:C:444:PHE:HA	1:C:447:LYS:HD3	1.93	0.50
1:C:1191:THR:HG22	1:C:1193:LYS:HG3	1.92	0.50
1:C:2339:GLU:HG3	1:D:2067:PHE:CE1	2.46	0.50
1:D:226:VAL:HG12	1:D:876:TRP:CE3	2.46	0.50
1:D:1410:GLY:HA3	1:D:1497:TYR:CE2	2.46	0.50
1:D:1523:LYS:HE2	1:D:1556:SER:H	1.76	0.50
1:D:1959:MET:HE2	1:D:1960:LEU:HD22	1.93	0.50
1:D:2063:GLN:O	1:D:2066:GLN:HG3	2.11	0.50
1:D:2192:SER:O	1:D:2195:VAL:HG22	2.09	0.50
1:E:158:GLU:HA	1:E:158:GLU:OE2	2.11	0.50
1:E:349:LEU:HG	1:E:414:LYS:CD	2.40	0.50
1:E:2364:ARG:NH1	1:E:2422:ILE:HG13	2.26	0.50
1:A:332:ILE:HD11	1:A:350:MET:CE	2.41	0.50
1:A:1197:LEU:HD23	1:A:1198:ARG:O	2.12	0.50
1:A:1378:MET:HE1	1:A:1393:PHE:CD2	2.46	0.50
1:C:136:TYR:HD1	1:C:141:ARG:HH12	1.59	0.50
1:D:475:GLN:HB3	1:D:477:ILE:HG23	1.94	0.50
1:D:504:GLN:HA	1:D:507:ASN:ND2	2.26	0.50
1:D:649:TRP:O	1:D:653:ALA:CB	2.59	0.50
1:E:968:TYR:CD1	1:E:974:ASP:HA	2.46	0.50
1:E:1127:ILE:O	1:E:1130:MET:HB3	2.10	0.50
1:E:1389:TYR:HA	1:E:1541:PHE:CZ	2.47	0.50
1:E:1507:THR:HG21	1:E:1541:PHE:HE1	1.75	0.50
1:E:2515:THR:HB	1:E:2516:ASP:HB2	1.93	0.50
1:A:458:SER:OG	1:A:460:LEU:HD23	2.10	0.50
1:A:491:PHE:CZ	1:A:495:ARG:HD2	2.47	0.50
1:A:1100:VAL:HB	1:A:1593:VAL:HG22	1.92	0.50
1:A:1319:LEU:HD12	1:A:1338:ILE:HD11	1.92	0.50
1:A:1513:ASP:HA	1:A:1574:LYS:HZ3	1.76	0.50
1:A:1629:GLN:HG2	1:A:1649:LEU:HD11	1.94	0.50
1:A:2328:TRP:CD2	1:A:2334:GLY:HA3	2.46	0.50
1:B:326:LYS:HG2	1:B:328:GLU:HB3	1.93	0.50
1:B:708:ILE:O	1:B:712:LEU:CB	2.55	0.50
1:B:899:VAL:HG22	1:B:902:LEU:O	2.10	0.50
1:C:482:VAL:O	1:C:486:VAL:HG23	2.10	0.50
1:D:2242:GLU:HA	1:D:2245:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:ASP:N	1:E:359:ILE:HG22	2.22	0.50
1:E:972:LEU:HD12	1:E:992:GLY:O	2.11	0.50
1:E:1158:ARG:HG3	1:E:1159:PRO:HD2	1.93	0.50
1:E:2277:THR:HA	1:E:2281:LEU:HD23	1.92	0.50
1:A:1408:LEU:HD22	1:A:1428:HIS:HB2	1.93	0.50
1:A:1839:TYR:CZ	1:A:1851:ASN:HB2	2.47	0.50
1:B:223:ASN:O	1:B:226:VAL:HG22	2.11	0.50
1:B:409:TYR:O	1:B:436:PHE:HB3	2.11	0.50
1:C:1342:THR:OG1	1:C:1353:THR:HB	2.11	0.50
1:C:1666:LYS:HE2	1:C:1703:SER:HA	1.93	0.50
1:C:2364:ARG:NH1	1:C:2422:ILE:HG13	2.26	0.50
1:D:1024:ASN:OD1	1:D:1030:TRP:HD1	1.94	0.50
1:D:1516:ILE:HD11	1:D:1569:ILE:HG23	1.92	0.50
1:E:2469:CYS:HB3	1:E:2495:PRO:HA	1.94	0.50
1:A:177:THR:HG23	1:A:179:GLY:H	1.76	0.50
1:A:1255:PHE:CD2	1:A:1285:SER:HA	2.47	0.50
1:A:2099:ILE:O	1:A:2103:GLN:HG2	2.12	0.50
1:B:848:ASP:OD2	1:B:850:SER:HB2	2.11	0.50
1:B:1084:PHE:HA	1:B:1087:VAL:HG12	1.94	0.50
1:B:1878:ASP:OD1	1:B:1880:MET:HG3	2.11	0.50
1:B:2372:TYR:HD2	1:B:2382:LEU:HD13	1.75	0.50
1:C:1363:TYR:OH	1:C:1507:THR:HG22	2.11	0.50
1:C:1438:LEU:HB2	1:C:1454:PHE:O	2.12	0.50
1:C:2453:ILE:HG13	1:C:2521:LEU:HD21	1.93	0.50
1:D:1063:ILE:HD12	1:D:1816:ARG:HG3	1.94	0.50
1:D:1123:ARG:HD2	1:D:1143:TRP:CZ2	2.47	0.50
1:D:2051:PRO:HA	1:D:2054:LEU:HD12	1.93	0.50
1:E:141:ARG:HH21	1:E:970:TYR:HA	1.76	0.50
1:E:1635:ASN:OD1	1:E:1636:THR:HG23	2.11	0.50
1:A:106:PRO:HA	1:A:1982:GLU:OE1	2.12	0.50
1:A:2454:ARG:HH21	1:A:2513:ASP:HB3	1.75	0.50
1:B:854:GLN:OE1	1:B:886:MET:HG3	2.12	0.50
1:B:1534:ALA:HB2	1:B:1548:PHE:C	2.36	0.50
1:C:776:LEU:HD11	1:C:814:HIS:HB2	1.93	0.50
1:D:1276:MET:HB2	1:D:1280:ALA:HB3	1.92	0.50
1:D:1333:MET:CE	1:D:1582:GLY:HA3	2.42	0.50
1:E:620:LEU:HB3	1:E:664:CYS:SG	2.52	0.50
1:E:1588:LEU:HD12	1:E:1589:SER:H	1.77	0.50
1:E:2052:VAL:HG21	1:E:2491:SER:HB2	1.92	0.50
1:A:76:SER:HB2	1:A:80:ARG:HE	1.77	0.50
1:A:76:SER:HB2	1:A:80:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:SER:HB2	1:A:557:ARG:HD3	1.92	0.50
1:A:806:THR:O	1:A:810:LEU:HD23	2.12	0.50
1:A:1304:LYS:HD3	1:A:1600:ILE:HD12	1.92	0.50
1:B:410:LYS:HE3	1:B:438:SER:H	1.76	0.50
1:B:1434:TYR:HB3	1:B:1487:ASN:ND2	2.27	0.50
1:B:1713:TYR:HD1	1:B:1718:TYR:CZ	2.30	0.50
1:C:297:LEU:HD23	1:C:297:LEU:H	1.76	0.50
1:C:330:TYR:HA	1:C:437:GLU:O	2.11	0.50
1:C:505:VAL:HG11	1:C:598:TYR:CD2	2.41	0.50
1:C:573:GLN:HA	1:C:576:LYS:HE2	1.93	0.50
1:C:901:ALA:O	1:C:902:LEU:HB2	2.12	0.50
1:C:2051:PRO:O	1:C:2054:LEU:HB2	2.12	0.50
1:D:349:LEU:HG	1:D:357:PHE:O	2.12	0.50
1:D:370:GLY:H	1:D:386:LEU:HB2	1.75	0.50
1:D:1132:ALA:HB1	1:D:1618:TYR:CZ	2.47	0.50
1:D:1167:HIS:HB3	1:D:1194:LEU:HD11	1.92	0.50
1:D:1666:LYS:N	1:D:1704:GLU:HG3	2.26	0.50
1:E:345:ASN:CG	1:E:362:ASN:HB2	2.37	0.50
1:E:636:LEU:O	1:E:640:VAL:HG23	2.12	0.50
1:E:1416:ASN:O	1:E:1420:ASN:CA	2.55	0.50
1:A:1643:THR:O	1:A:1647:GLN:HG3	2.11	0.50
1:A:2192:SER:OG	1:D:1149:ALA:HB2	2.12	0.50
1:B:25:LEU:CA	1:B:27:TYR:HB2	2.42	0.50
1:B:276:PHE:CD2	1:B:441:LEU:HD21	2.47	0.50
1:B:1508:GLY:C	1:B:1576:LYS:HE3	2.37	0.50
1:C:2145:ALA:HA	1:D:2210:ILE:HD11	1.94	0.50
1:D:1055:MET:HE3	1:D:1080:TYR:CE2	2.46	0.50
1:E:273:PRO:HG2	1:E:442:THR:HG22	1.92	0.50
1:A:1097:HIS:CE1	1:A:1127:ILE:HD11	2.47	0.50
1:A:1169:ILE:HD13	1:A:1194:LEU:HB2	1.94	0.50
1:A:1364:ASP:HB3	1:A:1371:ARG:NH1	2.26	0.50
1:A:1370:ILE:HD11	1:A:1397:ASN:O	2.12	0.50
1:A:2129:LYS:HZ2	1:A:2133:LEU:HB2	1.76	0.50
1:A:2363:THR:OG1	1:A:2533:ARG:HG2	2.12	0.50
1:B:498:LEU:HB3	1:B:502:ASP:HB2	1.93	0.50
1:B:1604:ARG:HB2	1:B:1612:TYR:CZ	2.47	0.50
1:B:2130:TYR:HE1	1:C:2225:ILE:HD12	1.77	0.50
1:C:858:SER:OG	1:C:891:ARG:HD2	2.12	0.50
1:C:2297:PHE:CE2	1:C:2328:TRP:HB2	2.47	0.50
1:C:2407:SER:O	1:C:2410:GLN:HG2	2.12	0.50
1:C:2434:ARG:HB2	1:C:2501:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LEU:HA	1:D:238:ILE:HG12	1.93	0.50
1:D:290:LEU:O	1:D:294:GLN:HG3	2.12	0.50
1:D:2155:GLN:NE2	1:E:2200:ALA:HB2	2.22	0.50
1:E:1287:LEU:HD11	1:E:1309:PHE:HB2	1.92	0.50
1:A:1050:ILE:HD11	1:A:1870:ASP:OD1	2.12	0.49
1:A:2450:TYR:CE1	1:E:2367:SER:HB2	2.47	0.49
1:B:870:ILE:O	1:B:874:LEU:HG	2.12	0.49
1:B:1265:MET:HE2	1:B:1265:MET:HA	1.94	0.49
1:B:1422:ILE:HG22	1:B:1466:PHE:HD2	1.77	0.49
1:C:207:ARG:HB3	1:C:211:MET:HE1	1.93	0.49
1:C:511:ILE:HD12	1:C:523:PHE:HD1	1.77	0.49
1:C:584:GLN:HG2	1:C:586:THR:HG23	1.92	0.49
1:C:1927:GLU:HB3	1:C:1991:TRP:CE2	2.46	0.49
1:D:2272:LEU:HG	1:D:2275:LYS:NZ	2.27	0.49
1:E:1839:TYR:CE1	1:E:1851:ASN:HB2	2.47	0.49
1:A:339:ASP:OD2	1:A:343:ASN:HB2	2.11	0.49
1:A:345:ASN:HD22	1:A:346:TYR:HB2	1.77	0.49
1:B:1350:LEU:HB3	1:B:1555:ALA:O	2.11	0.49
1:B:1443:VAL:HG11	1:B:1446:ASN:HB3	1.93	0.49
1:C:286:TYR:HB3	1:C:288:LEU:HD23	1.94	0.49
1:C:334:ARG:HD3	1:C:334:ARG:H	1.77	0.49
1:C:1073:VAL:HG11	1:C:1813:CYS:SG	2.52	0.49
1:C:1113:THR:HG23	1:C:1115:GLU:O	2.12	0.49
1:D:1387:SER:O	1:D:1388:GLN:HG2	2.12	0.49
1:E:52:GLU:HA	1:E:55:GLU:OE2	2.12	0.49
1:E:1831:ASN:HA	1:E:1834:TYR:O	2.13	0.49
1:E:2375:LEU:O	1:E:2379:ASN:HB3	2.12	0.49
1:A:676:ILE:HG23	1:A:679:LEU:HD23	1.94	0.49
1:A:750:ASN:HD22	1:A:753:GLU:HB3	1.77	0.49
1:A:1003:ARG:NH2	1:E:1838:GLY:HA3	2.27	0.49
1:A:2059:ASN:OD1	1:A:2060:LEU:HD12	2.12	0.49
1:A:2108:GLU:OE2	1:B:2246:ILE:HG23	2.11	0.49
1:B:70:ARG:HB3	1:B:85:ARG:HH22	1.77	0.49
1:B:239:LEU:HD12	1:B:487:PHE:HE1	1.76	0.49
1:B:484:THR:O	1:B:488:TYR:HD2	1.94	0.49
1:B:580:VAL:O	1:B:587:ILE:HD13	2.11	0.49
1:B:1456:PHE:HB3	1:B:1458:PRO:O	2.12	0.49
1:B:2322:PHE:HZ	1:B:2351:VAL:HG21	1.77	0.49
1:C:32:GLU:HB3	1:C:1011:ASP:HB2	1.94	0.49
1:C:827:THR:HA	1:C:830:MET:HG2	1.94	0.49
1:C:972:LEU:HD12	1:C:992:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1410:GLY:HA3	1:C:1497:TYR:HE2	1.78	0.49
1:D:290:LEU:O	1:D:293:VAL:HG22	2.11	0.49
1:E:235:LEU:HD23	1:E:487:PHE:CZ	2.47	0.49
1:E:331:LYS:HB2	1:E:437:GLU:HG2	1.94	0.49
1:E:356:GLN:O	1:E:402:SER:HA	2.12	0.49
1:E:1902:TYR:CD2	1:E:2007:ILE:HD13	2.46	0.49
1:E:2459:TYR:CZ	1:E:2461:GLY:HA3	2.48	0.49
1:A:986:LEU:O	1:A:990:ILE:HG12	2.11	0.49
1:A:2095:ALA:O	1:A:2099:ILE:HG12	2.12	0.49
1:B:628:THR:HA	1:B:631:LEU:HG	1.94	0.49
1:B:1788:TYR:OH	1:B:1791:PRO:HD3	2.13	0.49
1:B:1821:LYS:HE2	1:B:1821:LYS:HA	1.94	0.49
1:B:2163:SER:OG	1:B:2195:VAL:HG12	2.12	0.49
1:B:2423:PHE:CE1	1:B:2502:ASN:HB2	2.44	0.49
1:C:437:GLU:HG3	1:C:444:PHE:HZ	1.76	0.49
1:C:1140:TRP:CD1	1:C:1797:ALA:HA	2.48	0.49
1:C:2223:TRP:HA	1:C:2226:GLN:HE21	1.78	0.49
1:D:1234:GLY:O	1:D:1308:ARG:HG3	2.12	0.49
1:D:2453:ILE:HD12	1:D:2453:ILE:H	1.77	0.49
1:E:48:HIS:O	1:E:52:GLU:HG2	2.13	0.49
1:E:755:THR:HA	1:E:758:VAL:HG22	1.95	0.49
1:E:1024:ASN:OD1	1:E:1030:TRP:HD1	1.94	0.49
1:E:1821:LYS:NZ	1:E:1896:LEU:HD12	2.27	0.49
1:E:1885:ALA:O	1:E:1889:ARG:HG2	2.12	0.49
1:A:334:ARG:HB2	1:A:434:PHE:HA	1.93	0.49
1:A:336:LYS:HD2	1:A:430:GLY:C	2.37	0.49
1:A:998:ASN:HD21	1:E:1919:ARG:HG2	1.78	0.49
1:A:1662:PHE:HB2	1:A:1707:MET:SD	2.52	0.49
1:B:1078:LYS:HA	1:B:1078:LYS:HE3	1.94	0.49
1:B:1106:LEU:HD23	1:B:1108:TRP:CZ2	2.48	0.49
1:B:1158:ARG:HH11	1:B:1231:ALA:HA	1.77	0.49
1:B:1342:THR:OG1	1:B:1353:THR:HB	2.12	0.49
1:B:2045:LEU:HD22	1:B:2313:ARG:HG3	1.93	0.49
1:C:206:ILE:O	1:C:210:ILE:HG12	2.11	0.49
1:C:367:ARG:HA	1:C:390:LEU:HD21	1.93	0.49
1:C:2350:LYS:HB2	1:D:2299:LEU:HD11	1.94	0.49
1:C:2423:PHE:HE2	1:C:2502:ASN:HB2	1.77	0.49
1:D:220:LEU:O	1:D:227:MET:HE3	2.12	0.49
1:D:1148:THR:OG1	1:D:1150:VAL:HG23	2.12	0.49
1:D:1440:LEU:HD13	1:D:1482:ALA:HA	1.94	0.49
1:D:2332:THR:O	1:D:2335:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LEU:C	1:E:27:TYR:HB2	2.37	0.49
1:A:136:TYR:HD1	1:A:141:ARG:HH12	1.61	0.49
1:A:2279:LYS:HB2	1:E:2030:MET:HE2	1.94	0.49
1:A:2400:SER:C	1:A:2416:ARG:HH21	2.20	0.49
1:B:367:ARG:HD3	1:B:390:LEU:HD11	1.94	0.49
1:B:817:ILE:HD11	1:B:828:LEU:HD22	1.94	0.49
1:B:1287:LEU:O	1:B:1290:THR:HG22	2.12	0.49
1:C:91:SER:HB3	1:C:1960:LEU:HD11	1.95	0.49
1:C:217:LEU:O	1:C:220:LEU:HB3	2.13	0.49
1:C:274:GLU:HG2	1:C:1492:GLN:HA	1.94	0.49
1:C:1169:ILE:HD12	1:C:1193:LYS:O	2.13	0.49
1:C:1415:TYR:HB2	1:C:1476:PHE:CE2	2.47	0.49
1:C:2438:GLN:HG2	1:C:2494:LEU:HD21	1.95	0.49
1:D:297:LEU:HD23	1:D:297:LEU:H	1.77	0.49
1:D:986:LEU:O	1:D:990:ILE:HG12	2.12	0.49
1:D:1162:PHE:CD1	1:D:1241:LEU:HD21	2.48	0.49
1:D:1678:PHE:CD1	1:D:1699:LEU:HG	2.47	0.49
1:D:2163:SER:OG	1:D:2195:VAL:HG12	2.11	0.49
1:E:129:LEU:HD21	1:E:1018:PHE:CZ	2.48	0.49
1:E:336:LYS:HB3	1:E:415:ILE:HG21	1.94	0.49
1:E:616:MET:O	1:E:620:LEU:HG	2.13	0.49
1:E:2163:SER:OG	1:E:2195:VAL:HG12	2.13	0.49
1:E:2262:GLN:O	1:E:2265:THR:HG22	2.13	0.49
1:E:2328:TRP:CE2	1:E:2334:GLY:HA3	2.47	0.49
1:E:2423:PHE:CZ	1:E:2502:ASN:HB2	2.48	0.49
1:A:783:VAL:HG22	1:A:832:ARG:HE	1.78	0.49
1:A:1644:MET:O	1:A:1648:ARG:HG2	2.13	0.49
1:C:310:ALA:HB1	1:C:330:TYR:O	2.13	0.49
1:C:360:ARG:HE	1:C:365:VAL:HG13	1.77	0.49
1:C:1276:MET:HB2	1:C:1280:ALA:HB3	1.95	0.49
1:D:30:PHE:HD1	1:D:50:TYR:HD1	1.60	0.49
1:D:76:SER:HB3	1:D:80:ARG:HE	1.77	0.49
1:D:1130:MET:HE3	1:D:1133:GLY:H	1.78	0.49
1:D:2217:ARG:O	1:D:2221:GLN:HG2	2.12	0.49
1:E:318:GLY:HA2	1:E:329:ALA:HA	1.95	0.49
1:E:331:LYS:O	1:E:436:PHE:HA	2.13	0.49
1:E:443:ILE:HA	1:E:446:LEU:HD12	1.95	0.49
1:E:1440:LEU:HD13	1:E:1482:ALA:HA	1.94	0.49
1:A:437:GLU:HB2	1:A:439:TYR:HE2	1.77	0.49
1:B:1100:VAL:HB	1:B:1593:VAL:HG22	1.95	0.49
1:B:1436:ARG:HA	1:B:1487:ASN:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1763:GLY:O	1:B:1769:ILE:HA	2.13	0.49
1:B:2230:ALA:O	1:B:2234:VAL:HG23	2.12	0.49
1:B:2322:PHE:HE2	1:B:2348:MET:HA	1.78	0.49
1:C:225:GLU:HB2	1:C:875:GLN:OE1	2.13	0.49
1:C:331:LYS:O	1:C:436:PHE:HA	2.12	0.49
1:C:334:ARG:HH21	1:C:342:LYS:HD3	1.78	0.49
1:C:412:GLY:HA3	1:C:434:PHE:HD2	1.78	0.49
1:C:1678:PHE:CD1	1:C:1699:LEU:HG	2.48	0.49
1:D:1021:TRP:CH2	1:D:1025:ASN:HA	2.48	0.49
1:D:1431:ASN:HD22	1:D:1494:PHE:HZ	1.61	0.49
1:E:628:THR:HA	1:E:631:LEU:HG	1.94	0.49
1:E:1316:PRO:HD2	1:E:1588:LEU:HD11	1.94	0.49
1:E:1691:ARG:HD3	1:E:1735:ASP:OD2	2.13	0.49
1:E:2056:ARG:HA	1:E:2059:ASN:ND2	2.27	0.49
1:E:2297:PHE:HA	1:E:2300:THR:HG22	1.95	0.49
1:A:247:TYR:CZ	1:A:251:THR:HG21	2.47	0.49
1:A:1197:LEU:HB2	1:A:1203:TRP:CH2	2.48	0.49
1:A:1229:ALA:HB3	1:A:1246:TYR:CZ	2.47	0.49
1:A:1457:SER:HB2	1:A:1458:PRO:HD3	1.95	0.49
1:A:2052:VAL:O	1:A:2055:GLU:HG2	2.12	0.49
1:B:657:THR:O	1:B:660:ILE:HG22	2.13	0.49
1:B:1095:ALA:HA	1:B:1108:TRP:O	2.12	0.49
1:C:1046:PRO:O	1:C:1812:MET:HE1	2.13	0.49
1:D:356:GLN:O	1:D:402:SER:HA	2.12	0.49
1:D:357:PHE:HA	1:D:401:LEU:O	2.13	0.49
1:D:1191:THR:HG22	1:D:1193:LYS:HG3	1.94	0.49
1:D:1413:THR:OG1	1:D:1422:ILE:HG23	2.12	0.49
1:D:2230:ALA:O	1:D:2234:VAL:HG23	2.12	0.49
1:A:269:GLU:HG2	1:A:270:ASN:N	2.28	0.49
1:A:1639:ASP:HA	1:A:1832:TYR:HE2	1.77	0.49
1:A:1815:GLN:CG	1:A:1889:ARG:HH12	2.25	0.49
1:A:2484:PHE:HE2	1:E:2437:LYS:HZ1	1.58	0.49
1:B:1169:ILE:HD12	1:B:1193:LYS:O	2.13	0.49
1:B:1509:ILE:HD13	1:B:1575:ALA:HA	1.95	0.49
1:B:1515:LYS:HG2	1:B:1572:GLU:HB3	1.94	0.49
1:C:864:LEU:HD12	1:C:870:ILE:HG13	1.95	0.49
1:C:1651:GLU:OE1	1:C:1652:PRO:HD2	2.13	0.49
1:D:2423:PHE:CE2	1:D:2502:ASN:HB2	2.47	0.49
1:E:68:PHE:CD1	1:E:1981:PRO:HB3	2.48	0.49
1:E:780:GLU:HA	1:E:828:LEU:HD21	1.94	0.49
1:E:1415:TYR:HE1	1:E:1417:LYS:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1629:GLN:O	1:E:1633:ARG:HG2	2.13	0.49
1:E:1956:ASP:O	1:E:1960:LEU:HD23	2.13	0.49
1:E:2297:PHE:CE2	1:E:2328:TRP:HB2	2.47	0.49
1:A:1927:GLU:HB3	1:A:1991:TRP:CE2	2.47	0.48
1:B:345:ASN:OD1	1:B:362:ASN:HB2	2.12	0.48
1:B:1642:LEU:HD12	1:B:1832:TYR:CD2	2.48	0.48
1:B:2221:GLN:O	1:B:2225:ILE:HG12	2.12	0.48
1:B:2289:LEU:HD13	1:B:2292:ILE:HD11	1.95	0.48
1:C:452:ILE:HD12	1:C:455:CYS:SG	2.53	0.48
1:C:2405:LYS:HZ2	1:C:2407:SER:HB2	1.77	0.48
1:D:1169:ILE:HD12	1:D:1193:LYS:O	2.13	0.48
1:D:1229:ALA:HB3	1:D:1246:TYR:CZ	2.48	0.48
1:D:1898:GLY:HA3	1:D:1917:TYR:CE1	2.48	0.48
1:E:576:LYS:HG2	1:E:581:LEU:HD11	1.95	0.48
1:E:720:ALA:O	1:E:724:LEU:HG	2.12	0.48
1:E:1021:TRP:CH2	1:E:1025:ASN:HA	2.48	0.48
1:E:1265:MET:SD	1:E:1273:PHE:HB2	2.52	0.48
1:E:1457:SER:OG	1:E:1458:PRO:HD3	2.13	0.48
1:A:391:ILE:HG12	1:A:396:PHE:CZ	2.48	0.48
1:A:1172:GLU:HB2	1:A:1191:THR:HB	1.95	0.48
1:A:2056:ARG:HA	1:A:2059:ASN:HD21	1.77	0.48
1:B:1138:ASN:HB3	1:B:1862:ASN:ND2	2.28	0.48
1:C:347:PHE:HA	1:C:358:PHE:CE2	2.48	0.48
1:C:1927:GLU:HB3	1:C:1991:TRP:CD2	2.48	0.48
1:D:1409:GLY:HA3	1:D:1427:GLY:H	1.77	0.48
1:D:1932:GLY:HA2	1:D:1935:GLN:HE21	1.77	0.48
1:E:30:PHE:HE2	1:E:47:ARG:HA	1.78	0.48
1:E:216:THR:HG22	1:E:494:HIS:HB3	1.94	0.48
1:E:2049:ARG:HH21	1:E:2494:LEU:H	1.61	0.48
1:A:13:PRO:HD2	1:A:15:ARG:NH1	2.29	0.48
1:A:2484:PHE:CZ	1:E:2533:ARG:HD3	2.48	0.48
1:B:347:PHE:CD1	1:B:358:PHE:HZ	2.30	0.48
1:B:462:PRO:O	1:B:465:LEU:HG	2.13	0.48
1:B:1236:GLN:NE2	1:B:1308:ARG:HD3	2.28	0.48
1:C:181:SER:O	1:C:185:MET:HG2	2.13	0.48
1:C:1041:GLU:OE2	1:C:1881:HIS:HD2	1.96	0.48
1:C:1527:PHE:CD2	1:C:1551:LEU:HD13	2.48	0.48
1:C:2048:TYR:HA	1:C:2492:ARG:HA	1.95	0.48
1:D:129:LEU:HD11	1:D:1018:PHE:CE2	2.48	0.48
1:D:923:GLU:OE2	1:E:532:LEU:HD11	2.13	0.48
1:D:1197:LEU:HD12	1:D:1203:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1332:VAL:HG11	1:D:1362:ARG:HH21	1.78	0.48
1:D:1399:VAL:HA	1:D:1498:GLN:O	2.13	0.48
1:E:349:LEU:HB2	1:E:434:PHE:CZ	2.47	0.48
1:E:1351:ALA:HB1	1:E:1552:GLU:OE2	2.13	0.48
1:A:1532:HIS:HA	1:A:1549:LYS:HD2	1.95	0.48
1:A:1536:LEU:HD23	1:A:1536:LEU:H	1.76	0.48
1:A:2049:ARG:HH21	1:A:2494:LEU:H	1.60	0.48
1:A:2100:ARG:NH2	1:A:2104:ARG:HH21	2.12	0.48
1:B:1838:GLY:HA3	1:C:1003:ARG:NH2	2.27	0.48
1:C:897:ARG:H	1:C:908:ASN:HB3	1.77	0.48
1:C:1158:ARG:HH11	1:C:1231:ALA:HA	1.77	0.48
1:C:1626:LEU:HD23	1:C:1626:LEU:H	1.79	0.48
1:C:2230:ALA:O	1:C:2234:VAL:HG23	2.13	0.48
1:D:357:PHE:CD2	1:D:397:LYS:HE3	2.48	0.48
1:D:1527:PHE:CD2	1:D:1551:LEU:HD13	2.48	0.48
1:D:2142:GLU:O	1:D:2146:MET:HG2	2.13	0.48
1:D:2328:TRP:CE2	1:D:2334:GLY:HA3	2.49	0.48
1:D:2515:THR:C	1:D:2519:LYS:HB2	2.38	0.48
1:E:2359:ALA:HB1	1:E:2535:THR:HB	1.96	0.48
1:A:263:PHE:CE1	1:A:273:PRO:HD3	2.49	0.48
1:A:345:ASN:ND2	1:A:362:ASN:HB2	2.28	0.48
1:A:1626:LEU:HD23	1:A:1626:LEU:H	1.79	0.48
1:A:2186:GLY:HA2	1:A:2189:LEU:HD13	1.95	0.48
1:A:2198:LEU:HA	1:A:2201:THR:HG22	1.95	0.48
1:C:269:GLU:HG2	1:C:270:ASN:N	2.28	0.48
1:C:332:ILE:HG22	1:C:334:ARG:HD2	1.96	0.48
1:C:2465:MET:HE1	1:C:2469:CYS:HB2	1.94	0.48
1:D:359:ILE:HD11	1:D:395:ASN:HD21	1.78	0.48
1:D:1369:VAL:O	1:D:1373:LYS:HB2	2.13	0.48
1:D:2451:GLU:OE1	1:D:2453:ILE:HG13	2.13	0.48
1:E:130:HIS:HA	1:E:1009:ARG:HG3	1.95	0.48
1:E:848:ASP:OD2	1:E:850:SER:HB2	2.14	0.48
1:E:887:PRO:HA	1:E:890:ILE:HG12	1.96	0.48
1:E:1200:ASP:O	1:E:1200:ASP:OD2	2.30	0.48
1:E:1675:GLU:OE1	1:E:1963:GLY:HA2	2.14	0.48
1:E:1677:TRP:HZ3	1:E:1679:LYS:HG3	1.78	0.48
1:A:271:ILE:HG23	1:A:281:TRP:HZ2	1.78	0.48
1:A:1078:LYS:HA	1:A:1078:LYS:HE3	1.96	0.48
1:A:1510:ASN:H	1:A:1513:ASP:HB2	1.79	0.48
1:A:2129:LYS:HA	1:A:2129:LYS:HD2	1.69	0.48
1:B:336:LYS:HE3	1:B:431:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1438:LEU:HB2	1:B:1454:PHE:HB2	1.95	0.48
1:B:2443:LEU:HD12	1:B:2443:LEU:O	2.13	0.48
1:C:415:ILE:HD11	1:C:434:PHE:HD1	1.78	0.48
1:C:1059:LEU:HD12	1:C:1080:TYR:HB2	1.95	0.48
1:C:1082:THR:O	1:C:1085:GLU:HG3	2.13	0.48
1:C:1975:LEU:HG	1:C:1975:LEU:O	2.13	0.48
1:C:2250:ALA:O	1:C:2253:MET:HG2	2.13	0.48
1:D:416:TYR:HD1	1:D:431:GLY:HA3	1.78	0.48
1:D:1125:VAL:HB	1:D:1140:TRP:CE3	2.47	0.48
1:D:2099:ILE:HD13	1:D:2258:GLN:HB3	1.96	0.48
1:E:117:GLY:O	1:E:120:THR:HG22	2.13	0.48
1:E:184:LEU:O	1:E:188:LEU:HG	2.13	0.48
1:E:358:PHE:HD1	1:E:414:LYS:HZ1	1.61	0.48
1:E:676:ILE:HG12	1:E:758:VAL:HG12	1.96	0.48
1:E:910:PRO:HB3	1:E:914:GLU:CD	2.38	0.48
1:E:1839:TYR:CZ	1:E:1851:ASN:HB2	2.49	0.48
1:A:236:LEU:HD12	1:A:487:PHE:HB2	1.96	0.48
1:A:501:ASP:O	1:A:504:GLN:HG3	2.13	0.48
1:A:545:SER:HB2	1:A:586:THR:HG22	1.95	0.48
1:A:845:MET:HB3	1:A:847:LEU:HD23	1.96	0.48
1:A:1076:ALA:O	1:A:1079:THR:HG22	2.13	0.48
1:B:1919:ARG:HG2	1:C:998:ASN:HD21	1.77	0.48
1:B:2436:LEU:HD12	1:B:2501:VAL:HA	1.95	0.48
1:D:1839:TYR:CE1	1:D:1851:ASN:HB2	2.48	0.48
1:D:2099:ILE:O	1:D:2103:GLN:HG2	2.13	0.48
1:E:272:THR:HG22	1:E:275:ASN:OD1	2.14	0.48
1:E:332:ILE:HG12	1:E:436:PHE:HD1	1.79	0.48
1:E:1361:VAL:O	1:E:1543:ALA:HA	2.14	0.48
1:E:1897:ARG:HD3	1:E:1916:TRP:CZ2	2.49	0.48
1:E:2109:VAL:HG23	1:E:2247:ARG:HH21	1.78	0.48
1:E:2304:CYS:SG	1:E:2341:LEU:HD13	2.54	0.48
1:E:2308:GLN:NE2	1:E:2321:THR:HA	2.28	0.48
1:A:194:ALA:HB3	1:A:197:THR:HG23	1.95	0.48
1:A:336:LYS:HZ2	1:A:430:GLY:HA3	1.77	0.48
1:A:1415:TYR:HB2	1:A:1476:PHE:CE2	2.49	0.48
1:A:1439:ILE:HB	1:A:1483:VAL:HB	1.95	0.48
1:B:1331:THR:HG22	1:B:1332:VAL:H	1.79	0.48
1:B:1516:ILE:HD11	1:B:1569:ILE:HG23	1.96	0.48
1:B:2102:GLN:HB3	1:B:2254:GLN:HE22	1.79	0.48
1:C:200:HIS:O	1:C:203:TYR:HB3	2.13	0.48
1:C:331:LYS:HB2	1:C:437:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2486:LEU:HD11	1:C:2488:PHE:CZ	2.49	0.48
1:D:269:GLU:HG2	1:D:270:ASN:N	2.28	0.48
1:D:1055:MET:HG3	1:D:1083:ARG:HD2	1.95	0.48
1:D:1304:LYS:HD3	1:D:1600:ILE:HD12	1.94	0.48
1:D:1681:HIS:NE2	1:D:1726:GLY:HA3	2.29	0.48
1:E:70:ARG:HD3	1:E:83:ILE:HD11	1.96	0.48
1:E:332:ILE:HG12	1:E:436:PHE:CD1	2.48	0.48
1:E:739:GLY:HA2	1:E:742:THR:HG22	1.96	0.48
1:E:1422:ILE:HG12	1:E:1468:VAL:CG2	2.41	0.48
1:E:1641:ILE:HG22	1:E:1642:LEU:HD23	1.95	0.48
1:A:278:SER:HB3	1:A:281:TRP:HB3	1.95	0.48
1:A:1123:ARG:HD2	1:A:1143:TRP:CZ2	2.49	0.48
1:A:1865:PRO:HA	1:A:1873:ALA:HB1	1.96	0.48
1:A:1897:ARG:HD3	1:A:1916:TRP:CZ2	2.48	0.48
1:A:2104:ARG:HD2	1:B:2246:ILE:HD11	1.96	0.48
1:B:2137:ASP:OD2	1:B:2138:ILE:HG13	2.14	0.48
1:B:2371:PHE:CE1	1:B:2420:LEU:HD23	2.48	0.48
1:C:13:PRO:HD2	1:C:15:ARG:NH1	2.28	0.48
1:C:66:ARG:O	1:C:70:ARG:HG2	2.14	0.48
1:C:197:THR:OG1	1:C:198:PRO:HA	2.14	0.48
1:C:404:ILE:HG21	1:C:414:LYS:HG2	1.96	0.48
1:C:1125:VAL:HB	1:C:1140:TRP:CE3	2.49	0.48
1:C:1422:ILE:CG2	1:C:1466:PHE:HB2	2.44	0.48
1:D:206:ILE:HD11	1:D:919:ALA:HA	1.95	0.48
1:D:848:ASP:OD2	1:D:850:SER:HB2	2.14	0.48
1:D:1363:TYR:OH	1:D:1507:THR:HG22	2.14	0.48
1:E:1167:HIS:HB3	1:E:1194:LEU:HD11	1.96	0.48
1:E:2048:TYR:HA	1:E:2492:ARG:HA	1.96	0.48
1:A:130:HIS:HA	1:A:1009:ARG:HG3	1.95	0.48
1:A:216:THR:HG22	1:A:494:HIS:HB3	1.94	0.48
1:A:349:LEU:HD11	1:A:404:ILE:HG22	1.96	0.48
1:A:1409:GLY:HA3	1:A:1427:GLY:H	1.78	0.48
1:A:2178:LEU:HD21	1:B:2179:ALA:HB2	1.96	0.48
1:B:501:ASP:O	1:B:504:GLN:HG2	2.13	0.48
1:B:1085:GLU:HG2	1:B:1627:ALA:HB1	1.96	0.48
1:B:1227:ARG:HH12	1:B:1229:ALA:HB2	1.79	0.48
1:B:2439:VAL:HG23	1:B:2532:ILE:HG13	1.96	0.48
1:B:2442:THR:HA	1:B:2477:GLY:O	2.13	0.48
1:C:185:MET:HE2	1:C:201:GLN:OE1	2.13	0.48
1:C:468:ILE:HG22	1:C:482:VAL:HG13	1.95	0.48
1:C:1534:ALA:HB2	1:C:1548:PHE:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1814:PHE:HE1	1:C:1893:GLN:NE2	2.11	0.48
1:C:1882:TYR:O	1:C:1886:THR:HG23	2.13	0.48
1:C:2049:ARG:HG2	1:C:2493:TYR:CE1	2.48	0.48
1:C:2297:PHE:HA	1:C:2300:THR:HG22	1.95	0.48
1:D:522:HIS:HA	1:D:525:ARG:NH1	2.29	0.48
1:D:1831:ASN:HA	1:D:1834:TYR:O	2.14	0.48
1:D:2056:ARG:HA	1:D:2059:ASN:ND2	2.29	0.48
1:E:269:GLU:HG2	1:E:270:ASN:N	2.29	0.48
1:E:2241:LEU:O	1:E:2245:LYS:HG3	2.13	0.48
1:A:68:PHE:CD2	1:A:1981:PRO:HB3	2.49	0.47
1:A:1117:LEU:HD12	1:C:2164:ILE:HG23	1.96	0.47
1:A:2129:LYS:HG2	1:B:2225:ILE:HD11	1.96	0.47
1:A:2297:PHE:HA	1:A:2300:THR:HG22	1.95	0.47
1:B:1970:ARG:NH1	1:B:1971:THR:H	2.12	0.47
1:B:2322:PHE:CE2	1:B:2348:MET:HA	2.49	0.47
1:C:784:LEU:HB3	1:C:789:PHE:CE2	2.48	0.47
1:C:1487:ASN:H	1:C:1489:GLN:NE2	2.11	0.47
1:C:1487:ASN:H	1:C:1489:GLN:HE22	1.62	0.47
1:D:404:ILE:HG13	1:D:414:LYS:CD	2.44	0.47
1:D:1651:GLU:OE1	1:D:1652:PRO:HD2	2.13	0.47
1:D:1967:LYS:HG3	1:D:1968:ASN:N	2.29	0.47
1:D:1998:LEU:HD11	1:D:2002:ARG:NH1	2.29	0.47
1:E:547:ASP:HB3	1:E:550:GLU:HB2	1.95	0.47
1:E:689:GLU:HA	1:E:692:ALA:HB3	1.96	0.47
1:A:2100:ARG:HH21	1:A:2104:ARG:HH21	1.62	0.47
1:A:2174:ASN:ND2	1:B:2182:GLY:HA2	2.29	0.47
1:B:126:ALA:HB2	1:B:997:ILE:HD11	1.94	0.47
1:B:2409:ARG:HH21	1:B:2515:THR:HG21	1.78	0.47
1:C:601:THR:O	1:C:605:ARG:HG2	2.14	0.47
1:C:848:ASP:OD2	1:C:850:SER:HB2	2.14	0.47
1:C:2132:GLN:O	1:C:2136:GLU:HG2	2.14	0.47
1:D:439:TYR:HB2	1:D:444:PHE:CE1	2.49	0.47
1:D:1447:TYR:HB2	1:D:1491:PHE:CE1	2.48	0.47
1:E:930:GLN:O	1:E:934:LEU:HD23	2.15	0.47
1:E:1226:GLU:HG3	1:E:1247:LYS:HD2	1.95	0.47
1:E:1516:ILE:HD11	1:E:1569:ILE:CG2	2.44	0.47
1:E:1915:MET:O	1:E:1919:ARG:HG3	2.13	0.47
1:A:137:HIS:CD2	1:A:139:ASP:HB2	2.50	0.47
1:A:1288:LYS:HA	1:A:1291:PHE:HE1	1.77	0.47
1:B:845:MET:HB3	1:B:847:LEU:HD13	1.97	0.47
1:B:2174:ASN:HA	1:C:2185:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2251:ALA:O	1:B:2254:GLN:HG3	2.15	0.47
1:C:910:PRO:HD2	1:C:915:TRP:NE1	2.29	0.47
1:C:1635:ASN:OD1	1:C:1636:THR:HG23	2.14	0.47
1:C:1960:LEU:HD12	1:C:1960:LEU:HA	1.74	0.47
1:D:38:ASP:OD1	1:D:1585:LYS:HE3	2.14	0.47
1:D:2530:LEU:HB3	1:D:2532:ILE:HD11	1.96	0.47
1:E:1450:ARG:HD3	1:E:1452:PHE:O	2.13	0.47
1:E:1714:ALA:HB3	1:E:1717:TYR:CD2	2.50	0.47
1:E:2124:GLN:O	1:E:2127:LEU:HB3	2.14	0.47
1:A:126:ALA:HB2	1:A:997:ILE:HD11	1.96	0.47
1:A:657:THR:O	1:A:660:ILE:HG22	2.14	0.47
1:A:2360:LEU:HD11	1:B:2472:ILE:HA	1.96	0.47
1:B:1422:ILE:HG12	1:B:1468:VAL:CG2	2.42	0.47
1:B:1846:ALA:HB1	1:B:1848:TRP:CE2	2.49	0.47
1:B:2350:LYS:HD3	1:C:2299:LEU:CD1	2.44	0.47
1:C:27:TYR:HB3	1:C:28:LEU:HD22	1.95	0.47
1:C:2459:TYR:CZ	1:C:2461:GLY:HA3	2.49	0.47
1:D:247:TYR:CZ	1:D:251:THR:HG21	2.49	0.47
1:D:274:GLU:HB3	1:D:1405:TYR:CE1	2.44	0.47
1:D:335:VAL:H	1:D:433:ILE:HG22	1.78	0.47
1:D:2095:ALA:O	1:D:2099:ILE:HG12	2.14	0.47
1:E:373:LEU:HG	1:E:381:GLY:O	2.15	0.47
1:E:498:LEU:HD13	1:E:502:ASP:HB3	1.96	0.47
1:E:968:TYR:HD1	1:E:974:ASP:HA	1.78	0.47
1:E:1766:GLN:NE2	1:E:1767:GLN:HB2	2.29	0.47
1:A:233:ALA:HB1	1:A:898:TYR:HB3	1.97	0.47
1:A:336:LYS:HD2	1:A:431:GLY:N	2.29	0.47
1:A:468:ILE:HD11	1:A:500:PHE:CZ	2.44	0.47
1:B:841:LEU:O	1:B:845:MET:HG2	2.14	0.47
1:B:1122:TRP:HB3	1:B:1146:ILE:HD11	1.97	0.47
1:B:1241:LEU:HB2	1:B:1267:ILE:CG2	2.44	0.47
1:B:2088:LEU:HB3	1:B:2269:LEU:HD12	1.96	0.47
1:C:1046:PRO:C	1:C:1812:MET:HE1	2.39	0.47
1:C:2056:ARG:HA	1:C:2059:ASN:HD21	1.78	0.47
1:D:25:LEU:HA	1:D:27:TYR:HB2	1.96	0.47
1:D:27:TYR:CD2	1:D:28:LEU:HD22	2.49	0.47
1:D:250:LEU:HD11	1:D:454:LEU:HB3	1.95	0.47
1:D:2393:GLY:O	1:D:2406:LEU:HD22	2.15	0.47
1:E:791:VAL:HB	1:E:831:LEU:HD21	1.96	0.47
1:E:2230:ALA:O	1:E:2234:VAL:HG23	2.13	0.47
1:A:371:ALA:HA	1:A:382:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ASN:O	1:A:951:LEU:HG	2.15	0.47
1:A:1325:ILE:HA	1:A:1332:VAL:HG12	1.97	0.47
1:B:312:VAL:HG22	1:B:313:ASP:H	1.80	0.47
1:B:363:PHE:CZ	1:B:393:ASN:HA	2.49	0.47
1:C:1895:ILE:HD11	1:C:1994:LEU:HD11	1.95	0.47
1:D:86:ASP:OD1	1:D:88:VAL:HG12	2.15	0.47
1:D:972:LEU:HD12	1:D:992:GLY:O	2.14	0.47
1:D:2339:GLU:HA	1:D:2342:LEU:HD12	1.96	0.47
1:E:192:ARG:NH1	1:E:265:GLN:HB3	2.29	0.47
1:E:328:GLU:HB2	1:E:330:TYR:HB3	1.97	0.47
1:E:1523:LYS:NZ	1:E:1557:SER:H	2.12	0.47
1:A:360:ARG:NH1	1:A:365:VAL:HA	2.29	0.47
1:A:639:LEU:HG	1:A:643:LEU:HD23	1.97	0.47
1:A:1125:VAL:HB	1:A:1140:TRP:CE3	2.50	0.47
1:A:1997:ARG:NH1	1:A:2007:ILE:HD11	2.30	0.47
1:A:2196:MET:HE2	1:E:2155:GLN:O	2.15	0.47
1:A:2353:LEU:HD23	1:A:2353:LEU:HA	1.71	0.47
1:B:91:SER:HB3	1:B:1960:LEU:HD11	1.95	0.47
1:B:246:LEU:HD23	1:B:249:ILE:HD11	1.97	0.47
1:B:664:CYS:SG	1:B:803:ASN:HA	2.55	0.47
1:B:743:LEU:O	1:B:746:LYS:HB2	2.14	0.47
1:B:836:LEU:HD11	1:B:841:LEU:HD13	1.97	0.47
1:B:1096:TYR:HD1	1:B:1306:SER:HB2	1.80	0.47
1:B:1516:ILE:HD12	1:B:1570:VAL:O	2.15	0.47
1:B:1639:ASP:HA	1:B:1832:TYR:CE2	2.50	0.47
1:C:224:PRO:O	1:C:227:MET:HB2	2.14	0.47
1:C:334:ARG:NH2	1:C:342:LYS:HD3	2.30	0.47
1:C:344:ILE:HD11	1:C:429:GLN:HB3	1.96	0.47
1:C:374:ARG:HG3	1:C:380:SER:HB3	1.96	0.47
1:C:830:MET:HB2	1:C:835:THR:HG23	1.97	0.47
1:C:1096:TYR:HD1	1:C:1306:SER:HB2	1.79	0.47
1:C:1123:ARG:HD2	1:C:1143:TRP:CZ2	2.49	0.47
1:C:1265:MET:CA	1:C:1276:MET:HE1	2.44	0.47
1:C:1588:LEU:HD12	1:C:1589:SER:H	1.79	0.47
1:C:1720:HIS:ND1	1:C:1721:GLU:HG2	2.29	0.47
1:D:126:ALA:HB2	1:D:997:ILE:HD11	1.97	0.47
1:D:570:GLU:O	1:D:574:LEU:HD23	2.14	0.47
1:D:742:THR:O	1:D:746:LYS:HG2	2.14	0.47
1:D:901:ALA:O	1:D:902:LEU:HB2	2.14	0.47
1:D:1975:LEU:O	1:D:1975:LEU:HG	2.15	0.47
1:D:2051:PRO:O	1:D:2054:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2500:SER:HB3	1:D:2503:ASP:HB2	1.95	0.47
1:E:1235:PHE:HB3	1:E:1240:THR:HG22	1.96	0.47
1:E:2233:GLU:HA	1:E:2233:GLU:OE1	2.15	0.47
1:E:2410:GLN:HE22	1:E:2512:PRO:HG3	1.79	0.47
1:A:684:ARG:HG2	1:A:745:LEU:HA	1.96	0.47
1:A:2066:GLN:HA	1:A:2069:THR:HG22	1.97	0.47
1:A:2191:ALA:O	1:A:2195:VAL:HG13	2.15	0.47
1:A:2272:LEU:HD21	1:E:2083:LEU:CD1	2.43	0.47
1:A:2516:ASP:N	1:A:2519:LYS:HB2	2.27	0.47
1:B:158:GLU:HG3	1:B:982:LYS:CG	2.41	0.47
1:B:209:VAL:HG11	1:B:922:MET:HE1	1.96	0.47
1:B:347:PHE:HA	1:B:358:PHE:CZ	2.50	0.47
1:B:1132:ALA:HB1	1:B:1618:TYR:CZ	2.50	0.47
1:C:580:VAL:O	1:C:587:ILE:HD13	2.14	0.47
1:D:267:PHE:HB3	1:D:271:ILE:HB	1.96	0.47
1:D:1288:LYS:HA	1:D:1291:PHE:CD2	2.49	0.47
1:E:356:GLN:HE22	1:E:406:ASP:HA	1.79	0.47
1:E:501:ASP:O	1:E:504:GLN:HG2	2.15	0.47
1:E:969:SER:O	1:E:972:LEU:HD22	2.14	0.47
1:E:2253:MET:HA	1:E:2256:GLU:HG3	1.95	0.47
1:A:27:TYR:CD2	1:A:28:LEU:HD22	2.50	0.47
1:A:127:LYS:HB3	1:A:127:LYS:HE2	1.77	0.47
1:A:1678:PHE:CD1	1:A:1699:LEU:HG	2.50	0.47
1:A:1967:LYS:HG3	1:A:1968:ASN:N	2.30	0.47
1:A:2074:MET:C	1:A:2286:ARG:HH22	2.22	0.47
1:B:2284:TRP:HZ3	1:C:711:THR:HG22	1.80	0.47
1:B:2472:ILE:HG13	1:B:2473:ALA:H	1.79	0.47
1:C:350:MET:HE3	1:C:359:ILE:HD12	1.96	0.47
1:C:545:SER:HB2	1:C:586:THR:HG22	1.96	0.47
1:C:712:LEU:CD2	1:C:714:LEU:HB2	2.45	0.47
1:C:1515:LYS:HZ2	1:C:1572:GLU:HG3	1.80	0.47
1:C:2328:TRP:CE3	1:C:2334:GLY:HA3	2.50	0.47
1:C:2442:THR:HB	1:C:2529:ILE:HB	1.96	0.47
1:C:2458:ASN:O	1:C:2507:LEU:HD12	2.15	0.47
1:C:2515:THR:H	1:C:2516:ASP:CB	2.16	0.47
1:D:199:TYR:CD1	1:D:945:VAL:HG21	2.50	0.47
1:D:1516:ILE:HD12	1:D:1570:VAL:O	2.14	0.47
1:E:219:ALA:HB1	1:E:222:ARG:HH21	1.80	0.47
1:E:346:TYR:HD2	1:E:348:ASP:OD2	1.98	0.47
1:E:495:ARG:HE	1:E:496:TYR:HE1	1.63	0.47
1:E:1169:ILE:HD12	1:E:1193:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1523:LYS:HE2	1:E:1556:SER:H	1.80	0.47
1:A:296:TYR:CZ	1:A:462:PRO:HG3	2.50	0.47
1:A:332:ILE:HA	1:A:435:THR:O	2.15	0.47
1:A:464:GLU:O	1:A:467:THR:HG22	2.14	0.47
1:A:1516:ILE:HD12	1:A:1570:VAL:O	2.15	0.47
1:A:1572:GLU:OE2	1:A:1574:LYS:HB3	2.15	0.47
1:A:1902:TYR:CD1	1:A:2007:ILE:HD13	2.50	0.47
1:A:2335:LEU:O	1:A:2336:MET:HG3	2.15	0.47
1:B:324:GLU:HB3	1:B:351:TYR:CD2	2.50	0.47
1:C:1049:ARG:NH1	1:C:1056:MET:HE1	2.30	0.47
1:C:1648:ARG:HA	1:C:1853:ARG:NH1	2.30	0.47
1:C:1743:PHE:HE2	1:C:1784:ILE:HG12	1.79	0.47
1:C:2090:GLN:OE1	1:D:2264:HIS:HD2	1.98	0.47
1:D:451:ALA:O	1:D:454:LEU:HG	2.14	0.47
1:D:473:ASN:HD21	1:D:477:ILE:HG12	1.80	0.47
1:D:923:GLU:CD	1:E:532:LEU:HD11	2.40	0.47
1:D:2102:GLN:HB3	1:D:2254:GLN:HE22	1.79	0.47
1:E:286:TYR:HB3	1:E:288:LEU:HD23	1.97	0.47
1:E:1078:LYS:HA	1:E:1078:LYS:HE3	1.96	0.47
1:E:1534:ALA:HB2	1:E:1548:PHE:C	2.39	0.47
1:A:95:MET:HG3	1:A:96:PHE:CD2	2.50	0.46
1:B:68:PHE:CD2	1:B:1981:PRO:HB3	2.49	0.46
1:B:111:SER:HB3	1:B:114:SER:HB3	1.97	0.46
1:B:172:HIS:HA	1:B:175:ARG:NH1	2.30	0.46
1:B:328:GLU:HA	1:B:439:TYR:O	2.15	0.46
1:B:1411:PRO:HA	1:B:1425:VAL:O	2.16	0.46
1:B:2059:ASN:OD1	1:B:2060:LEU:HD12	2.15	0.46
1:B:2353:LEU:HA	1:B:2353:LEU:HD23	1.72	0.46
1:B:2436:LEU:HB2	1:B:2499:ILE:HG13	1.97	0.46
1:C:247:TYR:CZ	1:C:251:THR:HG21	2.50	0.46
1:C:1041:GLU:O	1:C:1044:ILE:HG22	2.15	0.46
1:C:1730:GLN:C	1:C:1732:ILE:H	2.22	0.46
1:D:1443:VAL:HG13	1:D:1446:ASN:H	1.81	0.46
1:D:1730:GLN:C	1:D:1732:ILE:H	2.22	0.46
1:D:1742:PHE:HB2	1:D:1756:ASN:ND2	2.30	0.46
1:D:2111:ALA:O	1:D:2115:VAL:HG23	2.14	0.46
1:E:356:GLN:NE2	1:E:409:TYR:HD1	2.13	0.46
1:E:660:ILE:HA	1:E:663:LEU:HD12	1.97	0.46
1:E:1041:GLU:OE2	1:E:1881:HIS:HD2	1.98	0.46
1:E:1083:ARG:HA	1:E:1086:THR:HG22	1.96	0.46
1:E:1743:PHE:HE2	1:E:1784:ILE:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.73	0.46
1:A:268:SER:HB2	1:A:271:ILE:HG13	1.97	0.46
1:A:1169:ILE:HD12	1:A:1193:LYS:O	2.16	0.46
1:A:1170:TRP:HE1	1:A:1193:LYS:HD3	1.79	0.46
1:A:2434:ARG:HB3	1:A:2536:ILE:HG22	1.95	0.46
1:B:195:ILE:HA	1:B:453:ARG:NH2	2.30	0.46
1:B:334:ARG:HH12	1:B:336:LYS:HB3	1.80	0.46
1:B:1677:TRP:HZ3	1:B:1679:LYS:HB2	1.81	0.46
1:B:1907:ARG:O	1:B:1910:LEU:HB3	2.15	0.46
1:B:2533:ARG:HD3	1:C:2484:PHE:CE1	2.50	0.46
1:C:15:ARG:HD3	1:C:15:ARG:N	2.29	0.46
1:C:194:ALA:O	1:C:197:THR:HG22	2.15	0.46
1:C:580:VAL:HG21	1:C:593:VAL:HG23	1.97	0.46
1:C:697:ARG:HA	1:C:700:GLN:OE1	2.14	0.46
1:C:1570:VAL:HG22	1:C:1585:LYS:HG2	1.96	0.46
1:C:2161:VAL:HG23	1:C:2162:LEU:HD22	1.97	0.46
1:D:310:ALA:CB	1:D:317:THR:HB	2.45	0.46
1:D:1163:ARG:O	1:D:1164:GLU:HG3	2.15	0.46
1:E:742:THR:O	1:E:746:LYS:HG2	2.15	0.46
1:E:1410:GLY:HA3	1:E:1497:TYR:CE2	2.46	0.46
1:E:1644:MET:HG3	1:E:1848:TRP:CE2	2.50	0.46
1:E:1725:LEU:HD23	1:E:1725:LEU:HA	1.77	0.46
1:E:2198:LEU:O	1:E:2201:THR:HG22	2.15	0.46
1:A:1156:ALA:HB3	1:A:1171:VAL:HG22	1.96	0.46
1:A:1647:GLN:HG2	1:A:1806:PHE:CE2	2.51	0.46
1:B:66:ARG:HG3	1:B:70:ARG:NH1	2.30	0.46
1:B:720:ALA:O	1:B:724:LEU:HG	2.15	0.46
1:B:2209:LYS:HB3	1:B:2209:LYS:HE3	1.52	0.46
1:C:319:LEU:HB2	1:C:330:TYR:CE1	2.51	0.46
1:C:523:PHE:HZ	1:C:538:GLU:HB2	1.80	0.46
1:C:2284:TRP:HB3	1:C:2288:LYS:NZ	2.30	0.46
1:D:360:ARG:HH21	1:D:366:SER:HB2	1.80	0.46
1:D:1644:MET:O	1:D:1648:ARG:HG2	2.16	0.46
1:D:2149:LEU:HD12	1:D:2149:LEU:HA	1.76	0.46
1:D:2178:LEU:HD21	1:E:2178:LEU:HD13	1.97	0.46
1:E:348:ASP:HB2	1:E:359:ILE:HG21	1.96	0.46
1:E:1268:TYR:HE1	1:E:1274:LYS:HD3	1.80	0.46
1:E:1678:PHE:CD1	1:E:1699:LEU:HG	2.50	0.46
1:E:2198:LEU:HA	1:E:2201:THR:HG22	1.97	0.46
1:A:235:LEU:HD23	1:A:487:PHE:HZ	1.80	0.46
1:A:779:ALA:HB3	1:E:2031:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1975:LEU:O	1:A:1975:LEU:HG	2.15	0.46
1:B:1092:VAL:HG12	1:B:1611:GLN:OE1	2.16	0.46
1:B:1131:GLN:HB2	1:B:1134:GLU:HG2	1.98	0.46
1:C:130:HIS:HA	1:C:1009:ARG:HG3	1.97	0.46
1:C:1276:MET:SD	1:C:1276:MET:N	2.88	0.46
1:C:1953:TYR:CE2	1:C:1957:LEU:HD11	2.50	0.46
1:D:8:LEU:HD11	1:D:20:MET:O	2.16	0.46
1:D:721:ARG:O	1:D:725:LEU:HG	2.16	0.46
1:D:2314:GLU:OE1	1:D:2315:LEU:HG	2.15	0.46
1:E:243:SER:H	1:E:246:LEU:HD12	1.79	0.46
1:E:1318:SER:C	1:E:1319:LEU:HD22	2.41	0.46
1:A:67:ILE:HD12	1:A:67:ILE:HA	1.83	0.46
1:A:566:VAL:HG22	1:A:567:ASN:O	2.15	0.46
1:A:899:VAL:HG22	1:A:902:LEU:O	2.16	0.46
1:A:1648:ARG:HA	1:A:1853:ARG:NH1	2.30	0.46
1:A:1821:LYS:HE3	1:A:1823:PHE:CZ	2.51	0.46
1:A:2366:VAL:HA	1:B:2450:TYR:HE2	1.80	0.46
1:B:984:THR:HG23	1:B:987:ALA:H	1.80	0.46
1:B:1439:ILE:HB	1:B:1483:VAL:HB	1.97	0.46
1:B:2410:GLN:HG3	1:B:2512:PRO:HA	1.96	0.46
1:B:2515:THR:C	1:B:2519:LYS:HB2	2.40	0.46
1:C:11:ILE:HA	1:C:40:GLN:OE1	2.15	0.46
1:C:201:GLN:HA	1:C:204:GLU:CD	2.40	0.46
1:C:460:LEU:HD21	1:C:468:ILE:HD12	1.98	0.46
1:C:1192:LEU:HB2	1:C:1211:ILE:HD13	1.98	0.46
1:C:1381:THR:HG21	1:C:1386:LYS:HA	1.98	0.46
1:C:1472:LYS:HB3	1:C:1475:ASP:HB3	1.96	0.46
1:C:2063:GLN:O	1:C:2066:GLN:HG3	2.16	0.46
1:D:250:LEU:HA	1:D:450:LYS:HZ1	1.81	0.46
1:D:596:SER:HA	1:D:599:ARG:HG2	1.97	0.46
1:D:1457:SER:HB3	1:D:1458:PRO:HD3	1.96	0.46
1:E:854:GLN:CD	1:E:886:MET:HE2	2.40	0.46
1:A:226:VAL:HG12	1:A:876:TRP:CD1	2.51	0.46
1:A:468:ILE:HG22	1:A:482:VAL:HG13	1.97	0.46
1:A:1059:LEU:HD12	1:A:1080:TYR:CB	2.46	0.46
1:A:1064:SER:OG	1:C:2210:ILE:HD13	2.16	0.46
1:A:1453:GLU:O	1:A:1453:GLU:HG2	2.16	0.46
1:A:1729:TYR:HB2	1:A:1732:ILE:HG23	1.97	0.46
1:A:1838:GLY:HA3	1:B:1003:ARG:NH2	2.31	0.46
1:B:722:TYR:HD1	1:B:725:LEU:HD12	1.79	0.46
1:C:336:LYS:HD3	1:C:415:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:LEU:HD23	1:C:1601:LEU:H	1.80	0.46
1:C:1666:LYS:N	1:C:1704:GLU:HG3	2.31	0.46
1:C:2075:ALA:HA	1:C:2286:ARG:HH21	1.81	0.46
1:D:207:ARG:HH21	1:D:240:ALA:HA	1.80	0.46
1:D:415:ILE:HD11	1:D:434:PHE:HD1	1.80	0.46
1:D:1082:THR:O	1:D:1085:GLU:HG3	2.16	0.46
1:D:1162:PHE:CD2	1:D:1241:LEU:HD21	2.50	0.46
1:D:1389:TYR:HA	1:D:1541:PHE:CZ	2.50	0.46
1:D:1431:ASN:ND2	1:D:1434:TYR:HB2	2.30	0.46
1:D:1891:LEU:HD11	1:D:1990:TYR:CD2	2.51	0.46
1:D:2242:GLU:O	1:D:2246:ILE:HG22	2.16	0.46
1:E:169:LEU:O	1:E:173:ILE:HG12	2.16	0.46
1:E:450:LYS:HA	1:E:453:ARG:CZ	2.46	0.46
1:E:1409:GLY:HA3	1:E:1427:GLY:CA	2.45	0.46
1:E:2483:GLN:NE2	1:E:2495:PRO:HG2	2.31	0.46
1:A:330:TYR:CD2	1:A:436:PHE:HE2	2.33	0.46
1:A:1574:LYS:HA	1:A:1581:LEU:H	1.81	0.46
1:A:2249:GLU:O	1:A:2253:MET:HG2	2.16	0.46
1:B:1234:GLY:O	1:B:1308:ARG:HG3	2.15	0.46
1:C:192:ARG:NH1	1:C:265:GLN:HG2	2.30	0.46
1:C:309:SER:HA	1:C:311:TYR:CE2	2.51	0.46
1:C:349:LEU:HD22	1:C:409:TYR:HD1	1.81	0.46
1:D:32:GLU:HB3	1:D:1011:ASP:HB2	1.96	0.46
1:D:775:ARG:HD3	1:D:775:ARG:HA	1.64	0.46
1:D:820:LEU:HB3	1:D:824:GLY:HA3	1.98	0.46
1:D:1288:LYS:HA	1:D:1291:PHE:CE2	2.51	0.46
1:D:1675:GLU:OE1	1:D:1963:GLY:HA2	2.16	0.46
1:D:2053:MET:HE1	1:D:2306:MET:HB3	1.96	0.46
1:E:247:TYR:HB2	1:E:898:TYR:OH	2.16	0.46
1:E:414:LYS:H	1:E:434:PHE:HB3	1.80	0.46
1:E:871:ASN:HA	1:E:874:LEU:HD12	1.98	0.46
1:E:1235:PHE:HB2	1:E:1242:LEU:HD11	1.98	0.46
1:E:1975:LEU:HG	1:E:1975:LEU:O	2.16	0.46
1:E:2064:LEU:HD12	1:E:2296:PHE:HD2	1.80	0.46
1:A:350:MET:HG3	1:A:359:ILE:HG13	1.98	0.46
1:A:742:THR:O	1:A:746:LYS:HG2	2.16	0.46
1:A:1026:ARG:CZ	1:A:1029:THR:HG21	2.45	0.46
1:A:1420:ASN:HB3	1:A:1468:VAL:HB	1.97	0.46
1:B:173:ILE:HD12	1:B:949:TRP:CZ3	2.51	0.46
1:B:350:MET:HB3	1:B:351:TYR:H	1.45	0.46
1:B:740:PHE:CD1	1:B:757:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:PHE:O	1:B:763:VAL:HG22	2.16	0.46
1:B:1725:LEU:HA	1:B:1725:LEU:HD23	1.77	0.46
1:B:2469:CYS:CB	1:B:2495:PRO:HA	2.45	0.46
1:B:2529:ILE:HD12	1:C:2450:TYR:HE1	1.81	0.46
1:C:290:LEU:HA	1:C:293:VAL:HG22	1.98	0.46
1:C:628:THR:HA	1:C:631:LEU:HG	1.96	0.46
1:C:1068:LEU:HD12	1:C:1073:VAL:HG22	1.97	0.46
1:C:2332:THR:HG21	1:C:2336:MET:HE1	1.98	0.46
1:D:436:PHE:HE2	1:D:438:SER:HB3	1.81	0.46
1:D:1068:LEU:HD23	1:D:1820:GLU:OE2	2.16	0.46
1:D:1390:GLY:HA2	1:D:1507:THR:C	2.41	0.46
1:D:1456:PHE:CZ	1:D:1461:ILE:HD12	2.51	0.46
1:D:1481:TYR:HD1	1:D:1498:GLN:HE22	1.64	0.46
1:D:2403:GLU:HB3	1:D:2405:LYS:HZ1	1.80	0.46
1:E:642:TRP:O	1:E:645:GLN:HG2	2.16	0.46
1:E:2048:TYR:CD2	1:E:2052:VAL:HG11	2.50	0.46
1:E:2222:GLU:O	1:E:2225:ILE:HG12	2.16	0.46
1:E:2513:ASP:HB3	1:E:2517:ARG:HG2	1.97	0.46
1:A:297:LEU:HD12	1:A:316:SER:HB2	1.97	0.46
1:A:613:GLU:HG3	1:A:657:THR:HG23	1.98	0.46
1:A:2116:LEU:HD12	1:A:2116:LEU:HA	1.77	0.46
1:B:1150:VAL:HG13	1:B:1170:TRP:CE2	2.51	0.46
1:B:1321:MET:HE3	1:B:1584:ILE:HD12	1.97	0.46
1:B:1678:PHE:CD1	1:B:1699:LEU:HG	2.50	0.46
1:D:1532:HIS:O	1:D:1548:PHE:HB3	2.16	0.46
1:E:513:GLN:HA	1:E:523:PHE:HB2	1.96	0.46
1:E:623:PHE:CD2	1:E:639:LEU:HD13	2.51	0.46
1:E:1810:PRO:HA	1:E:1829:TRP:HE1	1.81	0.46
1:A:119:LEU:HB2	1:A:990:ILE:HD11	1.98	0.46
1:A:130:HIS:CD2	1:A:1008:ALA:HA	2.51	0.46
1:A:330:TYR:HA	1:A:437:GLU:O	2.16	0.46
1:A:830:MET:HB2	1:A:835:THR:HG23	1.98	0.46
1:A:1162:PHE:CD2	1:A:1241:LEU:HD21	2.50	0.46
1:A:1162:PHE:CD2	1:A:1163:ARG:HG2	2.51	0.46
1:A:1651:GLU:OE1	1:A:1652:PRO:HD2	2.16	0.46
1:B:468:ILE:HD12	1:B:486:VAL:HG22	1.98	0.46
1:B:1476:PHE:HA	1:B:1479:CYS:SG	2.56	0.46
1:C:336:LYS:O	1:C:339:ASP:HB2	2.15	0.46
1:C:851:MET:HE1	1:D:567:ASN:ND2	2.31	0.46
1:C:1439:ILE:HG23	1:C:1450:ARG:CG	2.46	0.46
1:C:2058:ARG:O	1:C:2061:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:916:GLN:HG2	1:D:920:GLU:OE2	2.15	0.46
1:D:953:ASN:HB3	1:D:954:ILE:HD12	1.97	0.46
1:D:1400:LYS:O	1:D:1497:TYR:HA	2.16	0.46
1:E:1852:CYS:HB3	1:E:1855:LEU:HD12	1.98	0.46
1:A:27:TYR:HD2	1:A:28:LEU:HD22	1.81	0.45
1:A:137:HIS:HB3	1:A:140:ASN:HB2	1.98	0.45
1:A:224:PRO:HA	1:A:227:MET:HB2	1.98	0.45
1:A:353:GLY:HA3	1:A:397:LYS:HD2	1.98	0.45
1:B:547:ASP:HB3	1:B:550:GLU:HB2	1.98	0.45
1:B:1080:TYR:CZ	1:B:1809:THR:HG21	2.51	0.45
1:C:360:ARG:NE	1:C:365:VAL:HG13	2.30	0.45
1:C:373:LEU:HD12	1:C:416:TYR:CE2	2.51	0.45
1:C:1316:PRO:HD2	1:C:1588:LEU:HD11	1.98	0.45
1:C:2322:PHE:HA	1:C:2324:ARG:HH11	1.81	0.45
1:D:358:PHE:CE1	1:D:414:LYS:O	2.68	0.45
1:D:1662:PHE:HB2	1:D:1707:MET:SD	2.56	0.45
1:E:600:LEU:HD11	1:E:628:THR:HG21	1.98	0.45
1:E:1173:LYS:C	1:E:1173:LYS:HD3	2.41	0.45
1:A:1060:LEU:HA	1:A:1063:ILE:HG12	1.98	0.45
1:A:2213:SER:OG	1:D:1066:SER:HB3	2.16	0.45
1:A:2225:ILE:HG22	1:E:2129:LYS:HG2	1.97	0.45
1:A:2488:PHE:HB2	1:B:2485:MET:CE	2.42	0.45
1:B:194:ALA:HB1	1:B:948:ASN:OD1	2.17	0.45
1:B:200:HIS:HB3	1:B:203:TYR:HB3	1.98	0.45
1:B:776:LEU:HD12	1:B:780:GLU:HG3	1.98	0.45
1:B:1722:GLY:H	1:B:1766:GLN:CG	2.24	0.45
1:C:30:PHE:O	1:C:33:LEU:HB3	2.16	0.45
1:C:195:ILE:HG21	1:C:285:TYR:O	2.16	0.45
1:C:209:VAL:HA	1:C:212:THR:HG22	1.98	0.45
1:C:712:LEU:HD23	1:C:714:LEU:HB2	1.98	0.45
1:C:1173:LYS:O	1:C:1173:LYS:HG3	2.16	0.45
1:C:1378:MET:HE1	1:C:1393:PHE:CD1	2.51	0.45
1:C:2241:LEU:HD23	1:C:2245:LYS:HD2	1.98	0.45
1:D:327:LEU:HD12	1:D:327:LEU:O	2.15	0.45
1:D:387:SER:H	1:D:399:ASN:HB2	1.80	0.45
1:D:576:LYS:HG2	1:D:581:LEU:HD11	1.97	0.45
1:D:902:LEU:HB3	1:D:903:ASN:H	1.61	0.45
1:D:2101:ILE:O	1:D:2105:THR:HG23	2.16	0.45
1:D:2469:CYS:CB	1:D:2495:PRO:HA	2.43	0.45
1:E:225:GLU:HB2	1:E:875:GLN:OE1	2.17	0.45
1:E:708:ILE:O	1:E:712:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:736:ASP:HB3	1:E:739:GLY:H	1.81	0.45
1:E:1046:PRO:O	1:E:1812:MET:HE1	2.16	0.45
1:A:225:GLU:HB2	1:A:875:GLN:OE1	2.16	0.45
1:A:346:TYR:CE1	1:A:360:ARG:HD3	2.51	0.45
1:B:130:HIS:HA	1:B:1009:ARG:HG3	1.99	0.45
1:B:201:GLN:O	1:B:204:GLU:HG3	2.17	0.45
1:B:276:PHE:HA	1:B:281:TRP:CE3	2.51	0.45
1:B:776:LEU:HD11	1:B:814:HIS:HB2	1.99	0.45
1:B:1170:TRP:CE2	1:B:1193:LYS:HB2	2.51	0.45
1:B:1243:VAL:HG23	1:B:1265:MET:HB3	1.98	0.45
1:B:1399:VAL:CG1	1:B:1497:TYR:HB3	2.47	0.45
1:B:1827:THR:HA	1:B:1830:ILE:HG22	1.97	0.45
1:B:2124:GLN:O	1:B:2127:LEU:HB3	2.16	0.45
1:B:2350:LYS:HD3	1:C:2299:LEU:HD11	1.98	0.45
1:C:784:LEU:HB3	1:C:789:PHE:HE2	1.82	0.45
1:D:346:TYR:HA	1:D:361:ALA:H	1.80	0.45
1:E:462:PRO:O	1:E:465:LEU:HG	2.15	0.45
1:E:1123:ARG:HD2	1:E:1143:TRP:CZ2	2.51	0.45
1:E:1375:ILE:HG23	1:E:1379:LYS:NZ	2.32	0.45
1:E:1821:LYS:HA	1:E:1821:LYS:HD2	1.58	0.45
1:E:2438:GLN:HB3	1:E:2533:ARG:HB2	1.98	0.45
1:A:454:LEU:HD23	1:A:465:LEU:HD22	1.98	0.45
1:A:848:ASP:OD2	1:A:850:SER:HB2	2.16	0.45
1:A:2056:ARG:HA	1:A:2059:ASN:ND2	2.30	0.45
1:A:2372:TYR:HD2	1:A:2382:LEU:HD11	1.82	0.45
1:B:119:LEU:HD12	1:B:990:ILE:HG12	1.97	0.45
1:B:130:HIS:NE2	1:B:1008:ALA:HA	2.31	0.45
1:B:498:LEU:HD22	1:B:502:ASP:OD2	2.16	0.45
1:B:524:ASN:HA	1:B:528:ASN:HB2	1.98	0.45
1:B:2142:GLU:O	1:B:2146:MET:HG2	2.16	0.45
1:B:2375:LEU:O	1:B:2379:ASN:HB3	2.15	0.45
1:C:680:LEU:HB3	1:C:684:ARG:HE	1.80	0.45
1:C:1676:ARG:O	1:C:1699:LEU:HB2	2.15	0.45
1:D:26:GLN:N	1:D:27:TYR:HB2	2.31	0.45
1:E:334:ARG:HB2	1:E:433:ILE:O	2.16	0.45
1:E:2324:ARG:NH1	1:E:2324:ARG:HB2	2.32	0.45
1:E:2515:THR:CA	1:E:2516:ASP:HB2	2.46	0.45
1:A:334:ARG:CB	1:A:434:PHE:HA	2.47	0.45
1:A:842:ALA:HB2	1:A:852:VAL:HG21	1.99	0.45
1:A:1287:LEU:HA	1:A:1287:LEU:HD23	1.81	0.45
1:A:2235:LYS:HD2	1:E:2118:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2371:PHE:CE1	1:A:2420:LEU:HD13	2.52	0.45
1:B:349:LEU:HG	1:B:357:PHE:O	2.17	0.45
1:B:1162:PHE:CD2	1:B:1241:LEU:HD21	2.52	0.45
1:B:1195:ALA:HB2	1:B:1206:PRO:HB3	1.99	0.45
1:B:1632:SER:HB3	1:C:1164:GLU:OE2	2.16	0.45
1:B:1664:LEU:HB2	1:B:1705:THR:OG1	2.16	0.45
1:B:1960:LEU:HD12	1:B:1960:LEU:HA	1.76	0.45
1:C:1153:TYR:HE1	1:C:1154:LYS:HZ2	1.63	0.45
1:C:1507:THR:HG21	1:C:1541:PHE:HE1	1.81	0.45
1:C:1645:GLU:HG2	1:C:1646:THR:N	2.31	0.45
1:C:2052:VAL:HG12	1:C:2056:ARG:HE	1.81	0.45
1:C:2086:LEU:O	1:C:2090:GLN:HG3	2.16	0.45
1:D:130:HIS:HA	1:D:1009:ARG:HG3	1.98	0.45
1:D:191:TYR:HB3	1:D:197:THR:OG1	2.17	0.45
1:D:2323:ILE:HG13	1:D:2344:ASN:ND2	2.31	0.45
1:E:732:PRO:HG2	1:E:763:VAL:HG11	1.98	0.45
1:E:1324:ALA:O	1:E:1332:VAL:HG23	2.15	0.45
1:E:2154:GLY:O	1:E:2157:LEU:HG	2.16	0.45
1:A:359:ILE:HG21	1:A:361:ALA:HB2	1.99	0.45
1:A:360:ARG:CZ	1:A:365:VAL:HG22	2.46	0.45
1:A:387:SER:H	1:A:399:ASN:HB2	1.82	0.45
1:A:609:LEU:HG	1:A:613:GLU:CD	2.41	0.45
1:A:1063:ILE:O	1:A:1068:LEU:HD21	2.15	0.45
1:A:1236:GLN:NE2	1:A:1308:ARG:HD3	2.32	0.45
1:A:1884:ILE:O	1:A:1888:MET:HG2	2.16	0.45
1:A:2242:GLU:O	1:A:2246:ILE:HG13	2.17	0.45
1:B:226:VAL:HG21	1:B:879:VAL:HG21	1.98	0.45
1:B:404:ILE:HA	1:B:408:GLU:OE1	2.16	0.45
1:B:464:GLU:HG2	1:B:500:PHE:CD2	2.52	0.45
1:B:1351:ALA:HB1	1:B:1552:GLU:OE2	2.16	0.45
1:B:1454:PHE:HA	1:B:1455:PRO:HD3	1.79	0.45
1:B:1659:PHE:CE1	1:B:1710:PHE:HB2	2.51	0.45
1:B:1927:GLU:HB3	1:B:1991:TRP:CD2	2.51	0.45
1:B:2133:LEU:HA	1:B:2136:GLU:OE2	2.16	0.45
1:C:1150:VAL:HG13	1:C:1170:TRP:CE2	2.52	0.45
1:C:1478:LYS:HD2	1:C:1478:LYS:HA	1.71	0.45
1:D:30:PHE:HD1	1:D:50:TYR:CD1	2.34	0.45
1:D:346:TYR:CE1	1:D:360:ARG:HB3	2.51	0.45
1:D:532:LEU:HA	1:D:562:ARG:HH12	1.82	0.45
1:D:813:PHE:HD1	1:D:867:TRP:CD2	2.34	0.45
1:D:1287:LEU:O	1:D:1290:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:ARG:HH22	1:E:403:ASN:HB2	1.80	0.45
1:E:556:ALA:O	1:E:560:LEU:HD23	2.17	0.45
1:E:1287:LEU:HD23	1:E:1287:LEU:HA	1.76	0.45
1:E:1363:TYR:HB3	1:E:1375:ILE:CD1	2.47	0.45
1:A:48:HIS:O	1:A:52:GLU:OE1	2.35	0.45
1:A:202:PRO:O	1:A:206:ILE:HG12	2.17	0.45
1:A:247:TYR:HB2	1:A:898:TYR:OH	2.17	0.45
1:A:1827:THR:HA	1:A:1830:ILE:HG22	1.99	0.45
1:A:2230:ALA:O	1:A:2234:VAL:HG23	2.16	0.45
1:B:368:GLU:OE2	1:B:420:TYR:HB2	2.17	0.45
1:B:814:HIS:O	1:B:817:ILE:HG22	2.17	0.45
1:B:899:VAL:HG11	1:B:904:LYS:HB2	1.97	0.45
1:B:1304:LYS:HD3	1:B:1600:ILE:HD12	1.98	0.45
1:B:1624:THR:O	1:B:1625:LEU:HD23	2.16	0.45
1:B:1889:ARG:HA	1:B:1892:ASP:OD2	2.16	0.45
1:B:2111:ALA:O	1:B:2115:VAL:HG23	2.17	0.45
1:B:2113:ILE:HD11	1:B:2248:ARG:HB2	1.98	0.45
1:B:2410:GLN:HG3	1:B:2511:PHE:C	2.42	0.45
1:C:705:ALA:N	1:C:706:PRO:HD2	2.32	0.45
1:D:321:VAL:HG21	1:D:352:GLU:HG2	1.99	0.45
1:D:434:PHE:CG	1:D:435:THR:N	2.85	0.45
1:D:1350:LEU:HB3	1:D:1555:ALA:O	2.17	0.45
1:D:1838:GLY:HA3	1:E:1003:ARG:NH2	2.31	0.45
1:D:2130:TYR:CE2	1:D:2226:GLN:OE1	2.70	0.45
1:D:2407:SER:HB3	1:D:2412:GLU:OE2	2.17	0.45
1:D:2457:LEU:HB2	1:D:2472:ILE:HG22	1.99	0.45
1:E:28:LEU:HA	1:E:1015:ARG:HH21	1.81	0.45
1:E:192:ARG:HD2	1:E:265:GLN:O	2.17	0.45
1:E:1083:ARG:O	1:E:1086:THR:HG22	2.17	0.45
1:E:1084:PHE:HE1	1:E:1801:TYR:HB3	1.82	0.45
1:E:1399:VAL:HG13	1:E:1497:TYR:HB3	1.97	0.45
1:E:1439:ILE:HG23	1:E:1450:ARG:CG	2.43	0.45
1:E:2363:THR:OG1	1:E:2533:ARG:HG2	2.16	0.45
1:E:2515:THR:C	1:E:2519:LYS:HB2	2.42	0.45
1:A:372:THR:HG23	1:A:386:LEU:HD11	1.98	0.45
1:A:680:LEU:HD13	1:A:684:ARG:NH2	2.32	0.45
1:A:1932:GLY:CA	1:A:1935:GLN:HE21	2.30	0.45
1:A:2192:SER:O	1:A:2195:VAL:HG22	2.17	0.45
1:A:2275:LYS:HD3	1:E:2079:ASP:OD2	2.16	0.45
1:A:2442:THR:HA	1:A:2477:GLY:O	2.17	0.45
1:A:2469:CYS:HB3	1:A:2495:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:VAL:HA	1:B:1111:GLY:HA3	1.99	0.45
1:B:1389:TYR:HA	1:B:1541:PHE:CZ	2.52	0.45
1:B:2323:ILE:HG13	1:B:2344:ASN:ND2	2.31	0.45
1:C:38:ASP:OD1	1:C:1585:LYS:HE3	2.16	0.45
1:C:336:LYS:HD2	1:C:431:GLY:N	2.32	0.45
1:C:408:GLU:O	1:C:412:GLY:HA3	2.17	0.45
1:C:709:ALA:HB2	1:C:720:ALA:HB2	1.99	0.45
1:C:1009:ARG:O	1:C:1012:VAL:HG12	2.17	0.45
1:D:278:SER:HB3	1:D:281:TRP:HB2	1.98	0.45
1:D:317:THR:O	1:D:329:ALA:HA	2.17	0.45
1:D:744:VAL:HG22	1:D:757:LEU:HD21	1.98	0.45
1:D:1040:PRO:O	1:D:1044:ILE:HG12	2.17	0.45
1:D:1659:PHE:CE1	1:D:1710:PHE:HB2	2.52	0.45
1:D:1746:ASP:OD2	1:D:1749:LYS:HD3	2.17	0.45
1:D:2072:LEU:HD21	1:D:2335:LEU:HD13	1.99	0.45
1:E:489:THR:HA	1:E:503:ALA:HB1	1.99	0.45
1:E:1265:MET:CA	1:E:1276:MET:HE1	2.47	0.45
1:E:1633:ARG:HB3	1:E:1640:THR:HG22	1.99	0.45
1:A:48:HIS:O	1:A:51:HIS:HB2	2.16	0.45
1:A:191:TYR:CD2	1:A:197:THR:HG21	2.52	0.45
1:B:1437:ARG:NE	1:B:1437:ARG:HA	2.32	0.45
1:B:1645:GLU:HG2	1:B:1646:THR:N	2.31	0.45
1:B:1991:TRP:HB3	1:B:1995:ARG:HH12	1.81	0.45
1:B:2185:TRP:CH2	1:E:1174:GLU:HG2	2.52	0.45
1:C:1162:PHE:CD1	1:C:1241:LEU:HD21	2.52	0.45
1:C:1318:SER:HB2	1:C:1339:PRO:HA	1.98	0.45
1:C:1794:PHE:CZ	1:C:1854:PRO:HD3	2.51	0.45
1:C:2026:LEU:HD21	1:D:818:ASN:CG	2.42	0.45
1:C:2530:LEU:HD12	1:C:2532:ILE:HD11	1.99	0.45
1:D:39:ASP:OD1	1:D:40:GLN:HG3	2.16	0.45
1:D:111:SER:HB2	1:D:1982:GLU:HB2	1.98	0.45
1:D:141:ARG:HH21	1:D:970:TYR:HA	1.80	0.45
1:D:961:LEU:HD12	1:D:967:LEU:HD21	1.98	0.45
1:D:1436:ARG:HB2	1:D:1485:GLY:HA2	1.99	0.45
1:D:2494:LEU:HB3	1:D:2497:GLU:CD	2.41	0.45
1:E:349:LEU:HB2	1:E:434:PHE:CE2	2.52	0.45
1:E:366:SER:HB3	1:E:368:GLU:HB3	1.98	0.45
1:E:784:LEU:HB3	1:E:789:PHE:HE1	1.81	0.45
1:E:910:PRO:HB2	1:E:915:TRP:CD1	2.52	0.45
1:E:1162:PHE:CD2	1:E:1241:LEU:HD21	2.52	0.45
1:A:223:ASN:O	1:A:226:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD23	1:A:381:GLY:H	1.82	0.45
1:A:1108:TRP:CE2	1:A:1161:ILE:HD11	2.52	0.45
1:A:1405:TYR:HB2	1:A:1430:MET:HE1	1.99	0.45
1:B:359:ILE:CD1	1:B:361:ALA:HB2	2.47	0.45
1:B:679:LEU:O	1:B:683:LEU:HD23	2.16	0.45
1:B:1116:ASN:C	1:B:1117:LEU:HD22	2.42	0.45
1:B:2261:GLN:HA	1:B:2264:HIS:CE1	2.52	0.45
1:B:2358:ARG:HD2	1:C:2468:GLY:O	2.17	0.45
1:D:206:ILE:O	1:D:210:ILE:HG12	2.17	0.45
1:D:272:THR:HG22	1:D:275:ASN:ND2	2.30	0.45
1:D:468:ILE:HD11	1:D:485:LYS:HD3	1.98	0.45
1:D:2267:ALA:O	1:D:2270:GLU:HG2	2.16	0.45
1:E:650:LEU:CD1	1:E:655:ILE:HB	2.46	0.45
1:E:1168:LEU:O	1:E:1194:LEU:HD12	2.17	0.45
1:E:1395:ILE:HG22	1:E:1414:VAL:HG13	1.98	0.45
1:A:580:VAL:HG21	1:A:593:VAL:HG23	1.98	0.44
1:A:1266:THR:HG23	1:A:1274:LYS:HB2	1.99	0.44
1:A:2088:LEU:HB3	1:A:2269:LEU:HD12	1.99	0.44
1:A:2140:HIS:CB	1:A:2144:ARG:HH21	2.29	0.44
1:A:2270:GLU:HB2	1:E:2028:THR:HG21	1.99	0.44
1:A:2346:ALA:HB1	1:B:2299:LEU:HD23	1.98	0.44
1:B:194:ALA:HB3	1:B:197:THR:HG23	1.97	0.44
1:B:313:ASP:HB2	1:B:333:THR:HG23	1.98	0.44
1:B:1083:ARG:HG3	1:B:1083:ARG:HH11	1.82	0.44
1:B:1287:LEU:HA	1:B:1287:LEU:HD23	1.73	0.44
1:C:336:LYS:NZ	1:C:430:GLY:HA3	2.32	0.44
1:C:434:PHE:CZ	1:C:436:PHE:HB2	2.52	0.44
1:C:700:GLN:HA	1:C:703:ILE:HG12	2.00	0.44
1:C:1174:GLU:HB2	1:C:1189:ARG:HG2	1.98	0.44
1:C:1236:GLN:O	1:C:1236:GLN:HG3	2.17	0.44
1:C:1642:LEU:HD12	1:C:1832:TYR:CD2	2.52	0.44
1:C:1756:ASN:HB2	1:C:1774:LYS:O	2.18	0.44
1:C:2056:ARG:HA	1:C:2059:ASN:ND2	2.32	0.44
1:C:2284:TRP:HB3	1:C:2288:LYS:HZ1	1.82	0.44
1:D:42:SER:HB2	1:D:1568:ASP:OD1	2.17	0.44
1:D:58:LYS:HG2	1:D:1866:LEU:HD23	1.99	0.44
1:D:308:THR:HG22	1:D:309:SER:N	2.33	0.44
1:D:712:LEU:HD23	1:D:714:LEU:HB2	1.99	0.44
1:D:1839:TYR:CZ	1:D:1851:ASN:HB2	2.52	0.44
1:D:2120:ARG:HA	1:D:2237:MET:CE	2.43	0.44
1:E:1415:TYR:HB2	1:E:1476:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1439:ILE:HD13	1:E:1453:GLU:HA	2.00	0.44
1:E:1544:MET:HB3	1:E:1546:TYR:CE2	2.51	0.44
1:E:1809:THR:N	1:E:1810:PRO:HD2	2.32	0.44
1:E:2390:LEU:HD13	1:E:2523:GLU:HG2	1.98	0.44
1:E:2447:VAL:HG21	1:E:2453:ILE:HD11	1.99	0.44
1:A:676:ILE:HG13	1:A:758:VAL:HG12	1.98	0.44
1:A:917:THR:HA	1:A:920:GLU:OE1	2.17	0.44
1:A:1316:PRO:HD2	1:A:1588:LEU:HD11	1.98	0.44
1:A:1730:GLN:C	1:A:1732:ILE:H	2.25	0.44
1:A:2285:MET:HE2	1:A:2285:MET:HB2	1.82	0.44
1:A:2372:TYR:OH	1:A:2415:VAL:HG22	2.18	0.44
1:B:51:HIS:O	1:B:54:ILE:HG22	2.17	0.44
1:B:716:SER:OG	1:B:719:MET:HG3	2.18	0.44
1:B:812:ARG:HG2	1:B:812:ARG:HH11	1.82	0.44
1:B:1421:TYR:HD2	1:B:1467:THR:HA	1.82	0.44
1:B:2178:LEU:HD21	1:C:2178:LEU:HD13	1.99	0.44
1:C:748:SER:HB3	1:C:754:THR:HG21	1.99	0.44
1:C:835:THR:O	1:C:837:THR:HG23	2.17	0.44
1:C:953:ASN:HB3	1:C:954:ILE:HD12	1.99	0.44
1:C:1325:ILE:HD11	1:C:1366:SER:OG	2.17	0.44
1:C:1334:GLU:N	1:C:1334:GLU:OE2	2.50	0.44
1:C:1817:LEU:HD13	1:C:1825:GLU:HG2	1.99	0.44
1:C:1897:ARG:HD3	1:C:1916:TRP:CZ2	2.52	0.44
1:C:2142:GLU:HG2	1:C:2216:TYR:CE2	2.53	0.44
1:C:2154:GLY:O	1:C:2157:LEU:HB3	2.18	0.44
1:C:2219:ARG:HD3	1:C:2223:TRP:CZ2	2.52	0.44
1:C:2240:GLN:O	1:C:2244:LEU:HD23	2.17	0.44
1:D:217:LEU:HB3	1:D:220:LEU:CB	2.47	0.44
1:D:959:VAL:C	1:D:1400:LYS:HZ3	2.25	0.44
1:D:985:ARG:O	1:D:988:GLU:HG3	2.17	0.44
1:D:2442:THR:HB	1:D:2529:ILE:HB	1.99	0.44
1:E:358:PHE:HB2	1:E:401:LEU:HD23	1.99	0.44
1:E:724:LEU:O	1:E:737:ILE:HD11	2.17	0.44
1:E:1169:ILE:HD13	1:E:1194:LEU:HB2	1.98	0.44
1:E:2240:GLN:O	1:E:2244:LEU:HG	2.17	0.44
1:A:1387:SER:O	1:A:1388:GLN:HG2	2.17	0.44
1:A:1456:PHE:CE1	1:A:1461:ILE:HD13	2.52	0.44
1:A:1875:ALA:HB1	1:A:1882:TYR:CE1	2.52	0.44
1:A:2354:GLU:OE2	1:B:2306:MET:HE1	2.16	0.44
1:B:1055:MET:HE1	1:B:1084:PHE:HB2	1.99	0.44
1:B:2164:ILE:HG12	1:B:2195:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PHE:HA	1:C:358:PHE:CZ	2.52	0.44
1:C:464:GLU:O	1:C:468:ILE:HG13	2.16	0.44
1:C:807:LEU:HD12	1:C:808:PHE:N	2.32	0.44
1:C:1570:VAL:HA	1:C:1584:ILE:O	2.18	0.44
1:C:2095:ALA:O	1:C:2099:ILE:HG12	2.17	0.44
1:D:1415:TYR:HE1	1:D:1417:LYS:HA	1.82	0.44
1:D:1633:ARG:HB3	1:D:1640:THR:HG22	1.98	0.44
1:D:2389:PHE:CD1	1:D:2395:GLY:HA3	2.52	0.44
1:E:793:GLY:HA3	1:E:868:GLN:HG2	1.99	0.44
1:E:927:SER:OG	1:E:930:GLN:HG2	2.17	0.44
1:E:1967:LYS:HG3	1:E:1968:ASN:N	2.31	0.44
1:E:2336:MET:HE3	1:E:2336:MET:HB3	1.82	0.44
1:E:2407:SER:HB3	1:E:2412:GLU:OE2	2.17	0.44
1:A:334:ARG:HH21	1:A:342:LYS:CB	2.28	0.44
1:A:336:LYS:O	1:A:339:ASP:HB2	2.18	0.44
1:A:1084:PHE:HE2	1:A:1801:TYR:HB3	1.81	0.44
1:A:1662:PHE:CZ	1:A:1725:LEU:HD13	2.50	0.44
1:A:1692:GLN:OE1	1:A:1693:PRO:HD2	2.17	0.44
1:B:141:ARG:HH21	1:B:970:TYR:HA	1.82	0.44
1:B:482:VAL:O	1:B:486:VAL:HG23	2.17	0.44
1:B:660:ILE:HA	1:B:663:LEU:HB2	1.99	0.44
1:B:930:GLN:O	1:B:934:LEU:HD23	2.18	0.44
1:B:1628:SER:HB3	1:C:1163:ARG:HH21	1.83	0.44
1:B:2529:ILE:HD12	1:C:2450:TYR:CE1	2.53	0.44
1:C:365:VAL:HG11	1:C:390:LEU:HA	1.99	0.44
1:C:600:LEU:HD23	1:C:603:LEU:HD12	1.99	0.44
1:C:909:LEU:HA	1:C:910:PRO:HD3	1.89	0.44
1:C:1080:TYR:CE2	1:C:1809:THR:HG21	2.51	0.44
1:C:1823:PHE:O	1:C:1827:THR:HG23	2.18	0.44
1:C:1967:LYS:NZ	1:C:1968:ASN:H	2.16	0.44
1:C:2084:THR:O	1:C:2088:LEU:HD23	2.18	0.44
1:C:2125:ASN:ND2	1:D:2228:ASP:OD2	2.45	0.44
1:D:1321:MET:HG2	1:D:1584:ILE:HG21	1.99	0.44
1:D:1376:SER:HA	1:D:1379:LYS:HG3	1.99	0.44
1:D:1729:TYR:O	1:D:1730:GLN:HB2	2.18	0.44
1:D:1811:MET:HE2	1:D:1811:MET:HA	1.98	0.44
1:D:2065:THR:O	1:D:2069:THR:HG23	2.17	0.44
1:E:86:ASP:HB3	1:E:88:VAL:HG12	1.99	0.44
1:E:162:LEU:HD21	1:E:977:VAL:O	2.16	0.44
1:E:328:GLU:HB3	1:E:438:SER:HB2	1.98	0.44
1:E:1515:LYS:HZ2	1:E:1572:GLU:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1651:GLU:OE1	1:E:1652:PRO:HD2	2.18	0.44
1:A:332:ILE:CG2	1:A:334:ARG:HD2	2.45	0.44
1:A:595:SER:O	1:A:599:ARG:HG3	2.16	0.44
1:A:999:ARG:HH21	1:A:1005:GLU:HG2	1.81	0.44
1:A:1240:THR:C	1:A:1241:LEU:HD22	2.42	0.44
1:A:1645:GLU:HG2	1:A:1646:THR:N	2.33	0.44
1:A:1913:ALA:O	1:A:1917:TYR:HD2	2.01	0.44
1:A:2109:VAL:HG11	1:A:2248:ARG:HA	2.00	0.44
1:B:1021:TRP:CZ3	1:B:1025:ASN:HA	2.53	0.44
1:C:301:GLN:OE1	1:C:317:THR:HG23	2.18	0.44
1:C:680:LEU:HB3	1:C:684:ARG:HH21	1.83	0.44
1:C:959:VAL:HG13	1:C:961:LEU:HD22	1.99	0.44
1:C:1287:LEU:O	1:C:1290:THR:HG22	2.18	0.44
1:C:1621:ARG:NH2	1:C:1651:GLU:HB3	2.33	0.44
1:C:2140:HIS:CB	1:C:2144:ARG:HH21	2.30	0.44
1:D:676:ILE:O	1:D:680:LEU:HG	2.18	0.44
1:D:814:HIS:HA	1:D:817:ILE:HG12	1.98	0.44
1:D:1804:GLU:HA	1:D:1808:TYR:HD2	1.82	0.44
1:D:1927:GLU:HB3	1:D:1991:TRP:CD2	2.53	0.44
1:D:2308:GLN:CA	1:D:2348:MET:HE1	2.44	0.44
1:D:2442:THR:HA	1:D:2477:GLY:O	2.17	0.44
1:E:263:PHE:CE1	1:E:273:PRO:HD3	2.52	0.44
1:A:141:ARG:NH2	1:A:970:TYR:HA	2.32	0.44
1:A:839:ASP:HA	1:A:849:ILE:HD13	1.99	0.44
1:A:2161:VAL:HG23	1:A:2162:LEU:HD22	1.99	0.44
1:A:2198:LEU:O	1:A:2201:THR:HG22	2.17	0.44
1:B:129:LEU:HA	1:B:1012:VAL:HG11	2.00	0.44
1:B:1371:ARG:O	1:B:1375:ILE:HG22	2.17	0.44
1:B:1439:ILE:HD13	1:B:1453:GLU:HA	1.99	0.44
1:B:1457:SER:HB2	1:B:1458:PRO:HD3	1.98	0.44
1:C:610:THR:HG23	1:C:613:GLU:H	1.82	0.44
1:C:712:LEU:HD11	1:C:768:SER:HB3	2.00	0.44
1:C:743:LEU:HD13	1:C:753:GLU:OE1	2.17	0.44
1:C:813:PHE:HD1	1:C:867:TRP:CE3	2.34	0.44
1:C:1399:VAL:HG13	1:C:1497:TYR:HB3	2.00	0.44
1:C:2442:THR:HA	1:C:2477:GLY:O	2.18	0.44
1:C:2515:THR:HB	1:C:2516:ASP:OD2	2.18	0.44
1:D:462:PRO:O	1:D:465:LEU:HG	2.17	0.44
1:D:532:LEU:N	1:D:562:ARG:HH22	2.15	0.44
1:E:449:ASN:HA	1:E:452:ILE:HG22	2.00	0.44
1:E:663:LEU:HD21	1:E:769:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:CE2	1:A:251:THR:HG21	2.52	0.44
1:A:408:GLU:O	1:A:412:GLY:HA3	2.18	0.44
1:A:1148:THR:OG1	1:A:1150:VAL:HG23	2.18	0.44
1:A:1518:VAL:HG22	1:A:1569:ILE:HG12	1.98	0.44
1:B:498:LEU:HD13	1:B:502:ASP:HB3	1.98	0.44
1:B:1804:GLU:HA	1:B:1808:TYR:HD2	1.83	0.44
1:B:1975:LEU:O	1:B:1975:LEU:HD12	2.17	0.44
1:C:1122:TRP:HZ3	1:C:1124:ASN:ND2	2.16	0.44
1:C:1437:ARG:HA	1:C:1455:PRO:HA	2.00	0.44
1:C:1861:TRP:CE2	1:C:1876:GLN:HG2	2.53	0.44
1:D:271:ILE:HA	1:D:275:ASN:HD21	1.82	0.44
1:D:310:ALA:HB3	1:D:330:TYR:CZ	2.53	0.44
1:D:1713:TYR:HD1	1:D:1718:TYR:CZ	2.36	0.44
1:D:2529:ILE:HG12	1:E:2450:TYR:HE1	1.82	0.44
1:E:278:SER:OG	1:E:281:TRP:HB2	2.18	0.44
1:E:750:ASN:HB3	1:E:753:GLU:HB3	2.00	0.44
1:E:2453:ILE:H	1:E:2453:ILE:HD12	1.82	0.44
1:A:1515:LYS:HG2	1:A:1572:GLU:HB3	2.00	0.44
1:A:1777:LYS:HD3	1:A:1777:LYS:HA	1.76	0.44
1:A:1969:LEU:HG	1:A:1970:ARG:HG2	1.99	0.44
1:A:2144:ARG:HD3	1:E:1060:LEU:HD22	2.00	0.44
1:A:2417:LEU:HD21	1:A:2507:LEU:HB2	2.00	0.44
1:A:2436:LEU:HD23	1:A:2534:TYR:HB3	2.00	0.44
1:B:192:ARG:HD2	1:B:265:GLN:HG2	1.99	0.44
1:B:415:ILE:HG12	1:B:434:PHE:HB2	1.99	0.44
1:B:732:PRO:HD2	1:B:760:PHE:CE1	2.53	0.44
1:B:1220:ASP:O	1:B:1222:LYS:HG2	2.18	0.44
1:C:373:LEU:HD12	1:C:416:TYR:HE2	1.82	0.44
1:C:1240:THR:C	1:C:1241:LEU:HD22	2.43	0.44
1:C:1346:SER:OG	1:C:1349:ASN:HB2	2.17	0.44
1:C:2389:PHE:CD1	1:C:2395:GLY:HA3	2.52	0.44
1:D:250:LEU:HA	1:D:450:LYS:NZ	2.32	0.44
1:D:532:LEU:HG	1:D:533:LYS:HG3	1.99	0.44
1:D:696:ASN:ND2	1:D:699:LEU:HD22	2.33	0.44
1:D:1932:GLY:CA	1:D:1935:GLN:HE21	2.30	0.44
1:E:505:VAL:HG11	1:E:598:TYR:CD2	2.48	0.44
1:E:712:LEU:HD12	1:E:764:MET:HG2	1.99	0.44
1:E:830:MET:HA	1:E:835:THR:HG23	2.00	0.44
1:E:923:GLU:O	1:E:926:LEU:HG	2.17	0.44
1:A:129:LEU:HD21	1:A:1018:PHE:HZ	1.83	0.44
1:A:319:LEU:HD11	1:A:395:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:TRP:CD1	1:A:812:ARG:HH12	2.36	0.44
1:A:1226:GLU:HG3	1:A:1247:LYS:HD2	1.99	0.44
1:A:1338:ILE:O	1:A:1338:ILE:HG13	2.18	0.44
1:A:1539:ASN:HA	1:A:1544:MET:HE1	1.99	0.44
1:A:1960:LEU:HA	1:A:1964:GLY:HA2	1.99	0.44
1:A:1984:ASN:HB3	1:A:1987:LEU:HD23	1.99	0.44
1:B:1229:ALA:HB3	1:B:1246:TYR:CE2	2.53	0.44
1:B:1276:MET:HB2	1:B:1280:ALA:HB3	2.00	0.44
1:B:1431:ASN:HD22	1:B:1494:PHE:HZ	1.64	0.44
1:B:1518:VAL:HG11	1:B:1553:ILE:HG21	2.00	0.44
1:B:1888:MET:HE1	1:B:1990:TYR:CE2	2.53	0.44
1:B:2083:LEU:HD11	1:C:2272:LEU:HD12	1.99	0.44
1:B:2389:PHE:CD1	1:B:2395:GLY:HA3	2.53	0.44
1:C:346:TYR:O	1:C:358:PHE:HE2	2.01	0.44
1:C:606:VAL:HG23	1:C:607:HIS:ND1	2.32	0.44
1:C:902:LEU:HB3	1:C:903:ASN:H	1.61	0.44
1:C:1437:ARG:HG3	1:C:1454:PHE:C	2.42	0.44
1:C:1516:ILE:HD12	1:C:1570:VAL:O	2.18	0.44
1:D:28:LEU:HD12	1:D:32:GLU:CG	2.41	0.44
1:D:589:LEU:HD23	1:D:589:LEU:HA	1.88	0.44
1:D:679:LEU:HD23	1:D:711:THR:HG21	1.98	0.44
1:D:1156:ALA:HB3	1:D:1171:VAL:HG22	2.00	0.44
1:E:223:ASN:O	1:E:226:VAL:HG22	2.18	0.44
1:E:2472:ILE:HG13	1:E:2473:ALA:H	1.82	0.44
1:E:2494:LEU:HB3	1:E:2497:GLU:HG3	1.99	0.44
1:A:436:PHE:CZ	1:A:438:SER:HB3	2.52	0.43
1:A:2513:ASP:HA	1:A:2516:ASP:OD2	2.18	0.43
1:B:883:LEU:HB3	1:B:885:THR:HG22	1.99	0.43
1:B:1248:THR:HG22	1:B:1294:ILE:HG12	2.00	0.43
1:B:1648:ARG:HA	1:B:1853:ARG:NH1	2.33	0.43
1:B:2368:LEU:HD21	1:B:2530:LEU:HD11	2.00	0.43
1:C:2308:GLN:CA	1:C:2348:MET:HE1	2.48	0.43
1:D:59:ASN:O	1:D:63:LEU:HG	2.17	0.43
1:D:256:GLU:HG2	1:D:257:LYS:HD3	2.00	0.43
1:D:372:THR:OG1	1:D:401:LEU:HD11	2.18	0.43
1:E:141:ARG:NH2	1:E:970:TYR:HA	2.32	0.43
1:E:268:SER:H	1:E:271:ILE:HD12	1.83	0.43
1:E:439:TYR:HB3	1:E:440:PRO:O	2.17	0.43
1:E:813:PHE:HD1	1:E:867:TRP:CE3	2.36	0.43
1:E:1234:GLY:O	1:E:1308:ARG:HG3	2.18	0.43
1:E:1291:PHE:O	1:E:1293:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:HA	1:A:425:SER:O	2.18	0.43
1:A:676:ILE:HA	1:A:679:LEU:HB3	2.01	0.43
1:A:1277:GLU:H	1:A:1277:GLU:HG3	1.65	0.43
1:A:2193:ALA:O	1:A:2196:MET:HG3	2.18	0.43
1:B:87:SER:HA	1:B:90:ARG:HH11	1.83	0.43
1:B:217:LEU:HD12	1:B:220:LEU:HB2	2.00	0.43
1:B:225:GLU:HB2	1:B:875:GLN:OE1	2.18	0.43
1:B:387:SER:H	1:B:399:ASN:HB2	1.82	0.43
1:B:480:ASP:O	1:B:483:LEU:HG	2.18	0.43
1:B:1729:TYR:O	1:B:1730:GLN:HB2	2.18	0.43
1:B:1766:GLN:NE2	1:B:1767:GLN:HB2	2.33	0.43
1:C:268:SER:HB2	1:C:271:ILE:HG13	1.99	0.43
1:C:1049:ARG:HB3	1:C:1872:ASP:OD2	2.18	0.43
1:C:1520:ALA:HB1	1:C:1558:LEU:HD11	2.00	0.43
1:C:2101:ILE:O	1:C:2105:THR:HG23	2.18	0.43
1:C:2239:ALA:O	1:C:2242:GLU:HG3	2.17	0.43
1:D:68:PHE:CD2	1:D:1981:PRO:HB3	2.53	0.43
1:D:160:SER:HA	1:D:982:LYS:HA	1.99	0.43
1:D:524:ASN:HA	1:D:528:ASN:HD22	1.81	0.43
1:D:1078:LYS:HE3	1:D:1078:LYS:HA	2.00	0.43
1:D:1085:GLU:O	1:D:1089:ASP:HB2	2.18	0.43
1:E:169:LEU:HD23	1:E:169:LEU:HA	1.74	0.43
1:E:1413:THR:OG1	1:E:1422:ILE:HG23	2.18	0.43
1:E:1516:ILE:HD12	1:E:1570:VAL:O	2.18	0.43
1:E:1976:VAL:O	1:E:1976:VAL:HG13	2.18	0.43
1:A:25:LEU:CA	1:A:27:TYR:HB2	2.48	0.43
1:A:610:THR:HG23	1:A:613:GLU:H	1.84	0.43
1:A:687:ILE:HG13	1:A:745:LEU:HD21	2.00	0.43
1:A:1817:LEU:HD23	1:A:1817:LEU:HA	1.75	0.43
1:A:2097:GLN:O	1:A:2101:ILE:HG12	2.18	0.43
1:A:2225:ILE:HD12	1:E:2130:TYR:CZ	2.53	0.43
1:B:27:TYR:CD2	1:B:28:LEU:HB3	2.52	0.43
1:B:536:ILE:HD11	1:B:538:GLU:CD	2.44	0.43
1:B:618:TYR:HA	1:B:621:SER:HB3	1.99	0.43
1:B:899:VAL:HG21	1:B:904:LYS:HB2	1.99	0.43
1:B:1041:GLU:O	1:B:1044:ILE:HG22	2.18	0.43
1:B:1436:ARG:HA	1:B:1487:ASN:ND2	2.34	0.43
1:B:1626:LEU:HD13	1:B:1792:MET:HE1	1.99	0.43
1:C:235:LEU:HA	1:C:238:ILE:HG12	2.00	0.43
1:C:560:LEU:HD23	1:C:571:LEU:HD21	2.00	0.43
1:C:574:LEU:HD11	1:C:600:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2329:ASN:HD22	1:D:2288:LYS:NZ	2.16	0.43
1:D:360:ARG:HG2	1:D:398:SER:HB2	1.99	0.43
1:D:371:ALA:HB3	1:D:420:TYR:CE1	2.54	0.43
1:D:954:ILE:HG22	1:D:956:PRO:HD3	1.99	0.43
1:D:1255:PHE:CD2	1:D:1285:SER:HA	2.53	0.43
1:D:1852:CYS:HB3	1:D:1855:LEU:HD12	2.00	0.43
1:D:2045:LEU:HD23	1:D:2466:PRO:HD2	2.00	0.43
1:D:2353:LEU:HD23	1:D:2353:LEU:HA	1.73	0.43
1:E:1146:ILE:HG22	1:E:1148:THR:HG23	1.99	0.43
1:E:1891:LEU:CD1	1:E:1924:LEU:HD13	2.48	0.43
1:A:129:LEU:HA	1:A:1012:VAL:HG11	2.01	0.43
1:A:352:GLU:N	1:A:357:PHE:CZ	2.83	0.43
1:A:498:LEU:HB3	1:A:502:ASP:HB2	2.01	0.43
1:A:2079:ASP:OD1	1:B:2275:LYS:HD2	2.19	0.43
1:A:2422:ILE:HD12	1:A:2501:VAL:O	2.19	0.43
1:A:2522:LEU:O	1:A:2525:LEU:HB3	2.18	0.43
1:B:817:ILE:HA	1:B:820:LEU:HG	2.00	0.43
1:B:822:ASN:HB2	1:B:823:PRO:HD3	2.00	0.43
1:B:1068:LEU:HD23	1:B:1820:GLU:OE1	2.17	0.43
1:B:1115:GLU:CD	1:C:1204:SER:HB2	2.44	0.43
1:B:1277:GLU:CD	1:B:1278:ASN:H	2.26	0.43
1:B:1378:MET:HE1	1:B:1393:PHE:CG	2.54	0.43
1:B:2127:LEU:HD13	1:B:2231:ASP:HB3	1.99	0.43
1:B:2383:THR:HA	1:B:2386:LEU:HD12	2.00	0.43
1:C:199:TYR:CD1	1:C:945:VAL:HG21	2.53	0.43
1:C:226:VAL:HG12	1:C:876:TRP:NE1	2.32	0.43
1:C:1318:SER:C	1:C:1319:LEU:HD22	2.43	0.43
1:C:1825:GLU:O	1:C:1828:GLN:HG3	2.18	0.43
1:D:76:SER:HB3	1:D:80:ARG:NE	2.32	0.43
1:D:907:SER:OG	1:D:909:LEU:HD13	2.18	0.43
1:D:1108:TRP:CE2	1:D:1161:ILE:HD11	2.53	0.43
1:E:536:ILE:HD11	1:E:538:GLU:CD	2.43	0.43
1:E:1220:ASP:O	1:E:1222:LYS:HG2	2.18	0.43
1:E:1902:TYR:HE2	1:E:2007:ILE:HB	1.83	0.43
1:E:2140:HIS:CB	1:E:2144:ARG:HH21	2.32	0.43
1:E:2447:VAL:HG13	1:E:2451:GLU:HB2	2.00	0.43
1:A:345:ASN:ND2	1:A:364:LYS:HG3	2.34	0.43
1:A:415:ILE:HD11	1:A:434:PHE:CD1	2.53	0.43
1:A:415:ILE:HD11	1:A:434:PHE:HD1	1.82	0.43
1:A:1174:GLU:HG2	1:C:2185:TRP:CZ3	2.52	0.43
1:A:1342:THR:CG2	1:A:1353:THR:HB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:ASN:ND2	1:A:1530:SER:HA	2.33	0.43
1:B:1060:LEU:HD22	1:C:2144:ARG:HD3	2.00	0.43
1:B:1158:ARG:HG3	1:B:1159:PRO:HD2	2.00	0.43
1:B:1176:VAL:HB	1:B:1187:TYR:CZ	2.52	0.43
1:B:2053:MET:HE3	1:B:2307:ALA:HA	2.01	0.43
1:C:217:LEU:HD12	1:C:220:LEU:HB2	1.99	0.43
1:C:1809:THR:N	1:C:1810:PRO:HD2	2.33	0.43
1:C:2438:GLN:CG	1:C:2494:LEU:HD21	2.49	0.43
1:D:1476:PHE:HA	1:D:1479:CYS:HB2	1.99	0.43
1:D:1970:ARG:HH21	1:D:1973:ASN:HB3	1.83	0.43
1:D:2410:GLN:HG2	1:D:2412:GLU:OE2	2.18	0.43
1:D:2434:ARG:HB3	1:D:2536:ILE:HG22	2.01	0.43
1:D:2454:ARG:HH21	1:D:2513:ASP:HB3	1.83	0.43
1:E:194:ALA:HB3	1:E:197:THR:HG23	2.01	0.43
1:E:712:LEU:HD23	1:E:714:LEU:HB2	2.01	0.43
1:E:1957:LEU:HD23	1:E:1957:LEU:HA	1.82	0.43
1:E:1993:THR:O	1:E:1997:ARG:HG2	2.18	0.43
1:E:2328:TRP:CD2	1:E:2334:GLY:HA3	2.53	0.43
1:A:347:PHE:HA	1:A:358:PHE:CZ	2.54	0.43
1:A:1055:MET:HG3	1:A:1083:ARG:CD	2.48	0.43
1:A:1813:CYS:HB2	1:A:1829:TRP:NE1	2.33	0.43
1:A:1932:GLY:HA2	1:A:1935:GLN:HE21	1.83	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.85	0.43
1:B:768:SER:HA	1:B:771:VAL:HG12	2.01	0.43
1:B:1177:ALA:HB3	1:C:2176:PHE:HD1	1.84	0.43
1:B:1240:THR:C	1:B:1241:LEU:HD22	2.44	0.43
1:B:1265:MET:N	1:B:1276:MET:HE1	2.33	0.43
1:B:1766:GLN:HE21	1:B:1767:GLN:HB2	1.83	0.43
1:B:2251:ALA:O	1:B:2255:VAL:HG23	2.19	0.43
1:C:286:TYR:CZ	1:C:452:ILE:HG21	2.53	0.43
1:C:1050:ILE:HG13	1:C:1051:GLY:H	1.83	0.43
1:C:1084:PHE:HA	1:C:1087:VAL:HG12	2.01	0.43
1:D:194:ALA:O	1:D:197:THR:HG22	2.19	0.43
1:D:359:ILE:HG12	1:D:360:ARG:N	2.33	0.43
1:D:620:LEU:HD11	1:D:661:TRP:HA	2.01	0.43
1:D:712:LEU:CD2	1:D:714:LEU:HB2	2.49	0.43
1:D:1176:VAL:HB	1:D:1187:TYR:CZ	2.53	0.43
1:D:1336:GLY:HA2	1:D:1359:PHE:HB3	2.01	0.43
1:D:1425:VAL:HA	1:D:1463:ASN:HB3	2.00	0.43
1:D:1891:LEU:O	1:D:1894:LEU:HB2	2.18	0.43
1:D:1976:VAL:HG13	1:D:1976:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2108:GLU:OE2	1:E:2246:ILE:HG12	2.19	0.43
1:D:2297:PHE:CE2	1:D:2328:TRP:HB2	2.45	0.43
1:D:2436:LEU:HD12	1:D:2501:VAL:HA	2.00	0.43
1:E:437:GLU:HB2	1:E:439:TYR:CE2	2.53	0.43
1:E:663:LEU:HD22	1:E:770:SER:OG	2.19	0.43
1:E:840:ARG:HA	1:E:843:SER:OG	2.18	0.43
1:E:1240:THR:C	1:E:1241:LEU:HD22	2.44	0.43
1:A:365:VAL:HG21	1:A:390:LEU:O	2.19	0.43
1:A:702:GLU:HA	1:A:721:ARG:HG3	2.01	0.43
1:A:784:LEU:HB3	1:A:789:PHE:CE2	2.53	0.43
1:A:968:TYR:CD1	1:A:974:ASP:HA	2.54	0.43
1:A:1415:TYR:HB2	1:A:1476:PHE:CZ	2.53	0.43
1:A:1488:SER:C	1:A:1490:GLY:H	2.26	0.43
1:A:1718:TYR:CD2	1:A:1723:VAL:HB	2.53	0.43
1:A:1721:GLU:H	1:A:1766:GLN:HE21	1.64	0.43
1:A:2389:PHE:HA	1:A:2392:GLU:HG2	2.01	0.43
1:B:2299:LEU:HD12	1:B:2299:LEU:O	2.18	0.43
1:C:76:SER:HB3	1:C:80:ARG:NE	2.34	0.43
1:C:141:ARG:HH21	1:C:970:TYR:HA	1.84	0.43
1:C:2059:ASN:OD1	1:C:2060:LEU:HD12	2.19	0.43
1:C:2085:THR:O	1:C:2089:GLN:HG2	2.18	0.43
1:D:1678:PHE:HD1	1:D:1699:LEU:HG	1.82	0.43
1:D:1724:ARG:C	1:D:1725:LEU:HD12	2.44	0.43
1:D:1967:LYS:NZ	1:D:1968:ASN:H	2.17	0.43
1:E:104:VAL:HG11	1:E:110:ALA:HB3	2.01	0.43
1:E:580:VAL:O	1:E:587:ILE:HD13	2.18	0.43
1:E:663:LEU:O	1:E:802:HIS:CE1	2.72	0.43
1:E:1611:GLN:HG3	1:E:1623:ASN:ND2	2.33	0.43
1:E:1729:TYR:O	1:E:1730:GLN:HB2	2.19	0.43
1:A:10:LYS:HE2	1:A:40:GLN:O	2.19	0.43
1:A:505:VAL:HG21	1:A:598:TYR:HD2	1.82	0.43
1:A:535:LYS:NZ	1:A:536:ILE:HG22	2.33	0.43
1:A:2237:MET:HE2	1:A:2237:MET:HB2	1.87	0.43
1:B:113:PHE:HZ	1:B:1038:TYR:CD2	2.37	0.43
1:B:373:LEU:HG	1:B:381:GLY:O	2.19	0.43
1:B:414:LYS:HA	1:B:414:LYS:HD2	1.76	0.43
1:B:532:LEU:HD21	1:B:562:ARG:HD3	2.00	0.43
1:B:665:THR:HG23	1:B:667:GLU:H	1.84	0.43
1:B:1236:GLN:HE22	1:B:1308:ARG:HD3	1.82	0.43
1:B:1821:LYS:HD3	1:B:1823:PHE:CZ	2.54	0.43
1:B:1885:ALA:O	1:B:1888:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2101:ILE:O	1:B:2105:THR:HG23	2.18	0.43
1:B:2436:LEU:CD1	1:B:2501:VAL:HA	2.49	0.43
1:B:2457:LEU:CD1	1:B:2509:LEU:HG	2.48	0.43
1:C:410:LYS:HA	1:C:436:PHE:O	2.18	0.43
1:C:1197:LEU:HD13	1:C:1203:TRP:CZ2	2.53	0.43
1:C:1634:ALA:HB2	1:C:1641:ILE:HD11	1.99	0.43
1:C:1754:LEU:HD11	1:C:1757:ASP:HB3	2.00	0.43
1:C:2445:ALA:HB2	1:C:2525:LEU:HA	2.01	0.43
1:D:173:ILE:HD12	1:D:949:TRP:HZ3	1.84	0.43
1:D:369:PHE:HA	1:D:386:LEU:O	2.18	0.43
1:D:414:LYS:H	1:D:434:PHE:CB	2.32	0.43
1:D:1425:VAL:HG22	1:D:1463:ASN:HB3	2.00	0.43
1:D:2434:ARG:C	1:D:2501:VAL:HB	2.43	0.43
1:E:166:ASN:O	1:E:170:LEU:HG	2.19	0.43
1:E:372:THR:OG1	1:E:401:LEU:HD11	2.18	0.43
1:E:1817:LEU:HA	1:E:1817:LEU:HD23	1.86	0.43
1:A:158:GLU:HA	1:A:983:THR:O	2.19	0.43
1:A:475:GLN:HB2	1:A:477:ILE:HG12	2.01	0.43
1:A:948:ASN:C	1:A:948:ASN:HD22	2.26	0.43
1:A:1220:ASP:O	1:A:1222:LYS:HG2	2.19	0.43
1:A:1912:GLU:OE1	1:B:1026:ARG:HG2	2.19	0.43
1:A:2278:ASN:HB2	1:E:2030:MET:HE1	1.99	0.43
1:B:185:MET:HE3	1:B:185:MET:HB3	1.82	0.43
1:B:209:VAL:CG1	1:B:922:MET:HE1	2.49	0.43
1:B:1191:THR:HG22	1:B:1193:LYS:HG2	2.01	0.43
1:B:1563:ASN:HB3	1:B:1592:ARG:HB3	2.00	0.43
1:B:1823:PHE:O	1:B:1826:ALA:HB3	2.19	0.43
1:C:600:LEU:HD23	1:C:600:LEU:HA	1.84	0.43
1:C:1416:ASN:O	1:C:1420:ASN:HA	2.19	0.43
1:C:1518:VAL:HG21	1:C:1553:ILE:HD13	1.99	0.43
1:C:2434:ARG:HB3	1:C:2536:ILE:HG22	2.01	0.43
1:D:331:LYS:HE3	1:D:437:GLU:OE2	2.18	0.43
1:D:351:TYR:HB3	1:D:356:GLN:OE1	2.19	0.43
1:D:414:LYS:H	1:D:434:PHE:HB3	1.83	0.43
1:D:923:GLU:OE2	1:E:532:LEU:HD21	2.19	0.43
1:D:1342:THR:OG1	1:D:1353:THR:HB	2.19	0.43
1:D:2192:SER:HA	1:D:2195:VAL:HG22	2.00	0.43
1:D:2514:ALA:HB1	1:D:2522:LEU:HD12	2.00	0.43
1:E:1169:ILE:HD11	1:E:1192:LEU:HG	2.01	0.43
1:E:1197:LEU:HB2	1:E:1203:TRP:CH2	2.54	0.43
1:E:1331:THR:HG22	1:E:1363:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1489:GLN:CD	1:E:1492:GLN:HB2	2.43	0.43
1:E:1498:GLN:HE21	1:E:1499:SER:H	1.66	0.43
1:E:2186:GLY:HA2	1:E:2189:LEU:HD13	2.01	0.43
1:A:129:LEU:HD11	1:A:1018:PHE:CE2	2.54	0.43
1:A:132:SER:HA	1:A:137:HIS:CG	2.54	0.43
1:A:141:ARG:HH21	1:A:970:TYR:HA	1.84	0.43
1:A:352:GLU:H	1:A:357:PHE:HZ	1.67	0.43
1:A:1174:GLU:HB2	1:A:1189:ARG:CG	2.49	0.43
1:A:1442:PRO:HD3	1:A:1451:LEU:CG	2.47	0.43
1:A:1976:VAL:HG13	1:A:1976:VAL:O	2.19	0.43
1:A:2415:VAL:HG12	1:A:2420:LEU:HD21	2.01	0.43
1:B:334:ARG:HD2	1:B:415:ILE:HG13	2.01	0.43
1:B:827:THR:HG23	1:B:830:MET:HE3	2.00	0.43
1:B:1119:GLU:N	1:B:1119:GLU:OE2	2.52	0.43
1:B:1976:VAL:O	1:B:1976:VAL:HG13	2.19	0.43
1:B:2104:ARG:NE	1:B:2104:ARG:HA	2.33	0.43
1:C:698:GLU:OE2	1:C:699:LEU:HG	2.18	0.43
1:C:1095:ALA:HA	1:C:1108:TRP:O	2.19	0.43
1:C:1641:ILE:HG22	1:C:1642:LEU:HD23	2.01	0.43
1:C:2064:LEU:HD23	1:C:2296:PHE:HD2	1.83	0.43
1:C:2201:THR:HG22	1:C:2205:TYR:CE2	2.54	0.43
1:D:136:TYR:HD1	1:D:141:ARG:HH12	1.66	0.43
1:D:561:MET:HE3	1:D:568:SER:N	2.34	0.43
1:D:841:LEU:O	1:D:845:MET:HG2	2.19	0.43
1:D:1487:ASN:HB2	1:D:1489:GLN:HE22	1.84	0.43
1:D:1863:ALA:O	1:D:1865:PRO:HD3	2.19	0.43
1:D:2360:LEU:HD12	1:D:2360:LEU:HA	1.67	0.43
1:E:250:LEU:HD22	1:E:453:ARG:HE	1.84	0.43
1:E:1373:LYS:HE2	1:E:1412:ILE:HD13	2.00	0.43
1:E:1613:MET:HG2	1:E:1622:LEU:HD21	2.01	0.43
1:A:23:ALA:HB3	1:A:1955:GLN:OE1	2.18	0.42
1:A:26:GLN:N	1:A:27:TYR:HB2	2.34	0.42
1:A:601:THR:O	1:A:605:ARG:HG2	2.19	0.42
1:A:1106:LEU:HA	1:A:1106:LEU:HD12	1.83	0.42
1:A:2368:LEU:HD22	1:A:2528:ILE:HB	2.00	0.42
1:A:2393:GLY:O	1:A:2406:LEU:HD22	2.19	0.42
1:B:249:ILE:HA	1:B:252:GLU:OE2	2.19	0.42
1:B:484:THR:HG23	1:B:488:TYR:HE2	1.84	0.42
1:B:620:LEU:HB2	1:B:804:ILE:HD11	2.01	0.42
1:B:1049:ARG:H	1:B:1052:GLN:NE2	2.17	0.42
1:B:1059:LEU:HD12	1:B:1080:TYR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2109:VAL:HG11	1:B:2248:ARG:HA	2.00	0.42
1:B:2138:ILE:HG23	1:B:2142:GLU:HB2	2.01	0.42
1:B:2242:GLU:HA	1:B:2245:LYS:NZ	2.34	0.42
1:B:2448:GLY:H	1:B:2451:GLU:HG3	1.84	0.42
1:C:26:GLN:CB	1:C:27:TYR:HA	2.49	0.42
1:C:249:ILE:O	1:C:450:LYS:HE2	2.19	0.42
1:C:308:THR:HG21	1:C:359:ILE:HD11	2.00	0.42
1:C:414:LYS:HD2	1:C:414:LYS:HA	1.81	0.42
1:C:632:SER:OG	1:C:635:GLU:HB2	2.19	0.42
1:C:968:TYR:CD1	1:C:974:ASP:HA	2.54	0.42
1:C:2350:LYS:HD3	1:D:2299:LEU:HD13	2.00	0.42
1:C:2519:LYS:HE3	1:C:2519:LYS:HB3	1.93	0.42
1:D:308:THR:HG23	1:D:395:ASN:HD21	1.84	0.42
1:D:649:TRP:O	1:D:653:ALA:HB3	2.19	0.42
1:D:813:PHE:O	1:D:817:ILE:HG23	2.19	0.42
1:D:1684:ASN:O	1:D:1723:VAL:HG23	2.19	0.42
1:D:2410:GLN:HB2	1:D:2512:PRO:HA	2.00	0.42
1:E:158:GLU:OE1	1:E:982:LYS:HE2	2.19	0.42
1:E:308:THR:HG23	1:E:395:ASN:ND2	2.34	0.42
1:E:557:ARG:HH21	1:E:561:MET:HE2	1.84	0.42
1:E:1122:TRP:HB3	1:E:1146:ILE:HD11	2.01	0.42
1:E:1627:ALA:O	1:E:1631:VAL:HG23	2.17	0.42
1:A:76:SER:HB2	1:A:80:ARG:NE	2.34	0.42
1:A:142:ARG:HE	1:A:142:ARG:HB3	1.73	0.42
1:A:373:LEU:HG	1:A:381:GLY:O	2.19	0.42
1:A:1092:VAL:HG21	1:A:1109:PHE:CD2	2.54	0.42
1:A:1211:ILE:O	1:A:1215:VAL:HG12	2.19	0.42
1:A:1334:GLU:OE2	1:A:1335:ASN:HB2	2.19	0.42
1:B:234:SER:O	1:B:238:ILE:HG12	2.19	0.42
1:B:558:SER:O	1:B:561:MET:HB2	2.20	0.42
1:B:1226:GLU:OE1	1:B:1247:LYS:HD3	2.19	0.42
1:B:1927:GLU:HB3	1:B:1991:TRP:CE2	2.54	0.42
1:C:346:TYR:CE1	1:C:362:ASN:HB2	2.54	0.42
1:C:577:LEU:HD13	1:C:615:CYS:SG	2.59	0.42
1:C:2192:SER:O	1:C:2195:VAL:HG22	2.17	0.42
1:D:818:ASN:ND2	1:D:2274:ARG:HH21	2.17	0.42
1:D:1431:ASN:HB2	1:D:1494:PHE:CZ	2.54	0.42
1:D:1507:THR:HG21	1:D:1541:PHE:HE1	1.84	0.42
1:E:412:GLY:HA3	1:E:434:PHE:CD2	2.49	0.42
1:E:2146:MET:HG2	1:E:2146:MET:H	1.67	0.42
1:E:2469:CYS:CB	1:E:2495:PRO:HA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:HB3	1:A:281:TRP:NE1	2.34	0.42
1:A:485:LYS:O	1:A:489:THR:HG23	2.19	0.42
1:A:975:ASN:C	1:A:976:GLN:HG3	2.44	0.42
1:A:1276:MET:SD	1:A:1276:MET:N	2.91	0.42
1:A:2184:ARG:HH21	1:B:2184:ARG:HH12	1.66	0.42
1:B:162:LEU:HD21	1:B:977:VAL:O	2.18	0.42
1:B:835:THR:HB	1:B:840:ARG:HH12	1.84	0.42
1:B:2116:LEU:HD21	1:B:2240:GLN:HB3	2.01	0.42
1:B:2223:TRP:O	1:B:2226:GLN:HG3	2.20	0.42
1:C:69:THR:HG22	1:C:1880:MET:HE1	2.01	0.42
1:C:816:TRP:CE3	1:C:867:TRP:CZ3	3.07	0.42
1:C:1676:ARG:HB2	1:C:1698:MET:SD	2.58	0.42
1:C:1804:GLU:HA	1:C:1808:TYR:HB2	2.01	0.42
1:C:1923:LEU:HD23	1:C:1923:LEU:O	2.19	0.42
1:C:1967:LYS:HA	1:C:1967:LYS:HD2	1.73	0.42
1:C:2267:ALA:O	1:C:2270:GLU:HG2	2.19	0.42
1:C:2353:LEU:HD23	1:C:2353:LEU:HA	1.73	0.42
1:D:310:ALA:HB2	1:D:317:THR:HB	2.01	0.42
1:D:2281:LEU:O	1:D:2285:MET:HG2	2.20	0.42
1:E:1691:ARG:HD3	1:E:1735:ASP:CG	2.44	0.42
1:A:416:TYR:CD1	1:A:431:GLY:HA3	2.49	0.42
1:A:1319:LEU:HB2	1:A:1338:ILE:HD11	2.02	0.42
1:A:1437:ARG:O	1:A:1439:ILE:HG12	2.18	0.42
1:A:1666:LYS:N	1:A:1704:GLU:HG3	2.34	0.42
1:A:1815:GLN:HE21	1:A:1889:ARG:HH22	1.67	0.42
1:A:1902:TYR:CE1	1:A:2007:ILE:HD13	2.54	0.42
1:A:2437:LYS:NZ	1:B:2484:PHE:HE2	2.17	0.42
1:A:2455:ALA:HB2	1:A:2511:PHE:HE1	1.84	0.42
1:B:311:TYR:CE2	1:B:342:LYS:HD3	2.54	0.42
1:B:404:ILE:HG22	1:B:408:GLU:OE1	2.20	0.42
1:B:1132:ALA:HB1	1:B:1618:TYR:OH	2.20	0.42
1:B:1891:LEU:O	1:B:1894:LEU:HB2	2.19	0.42
1:B:2198:LEU:O	1:B:2201:THR:HG22	2.18	0.42
1:B:2222:GLU:OE1	1:B:2222:GLU:HA	2.19	0.42
1:B:2364:ARG:NH1	1:B:2422:ILE:HG12	2.34	0.42
1:C:719:MET:HE1	1:C:778:GLU:HA	2.02	0.42
1:C:1604:ARG:HE	1:C:1604:ARG:HB3	1.64	0.42
1:C:1713:TYR:HD1	1:C:1718:TYR:CZ	2.36	0.42
1:C:2099:ILE:O	1:C:2103:GLN:HG2	2.19	0.42
1:C:2196:MET:HA	1:C:2196:MET:HE2	2.01	0.42
1:C:2261:GLN:HA	1:C:2264:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2483:GLN:NE2	1:C:2495:PRO:HG2	2.34	0.42
1:D:386:LEU:H	1:D:386:LEU:HD12	1.83	0.42
1:E:1612:TYR:HB2	1:E:1620:ILE:O	2.19	0.42
1:E:1856:GLU:CD	1:E:1856:GLU:C	2.88	0.42
1:E:2116:LEU:HD12	1:E:2116:LEU:HA	1.78	0.42
1:A:217:LEU:O	1:A:220:LEU:HB3	2.19	0.42
1:A:370:GLY:N	1:A:386:LEU:HB2	2.31	0.42
1:A:580:VAL:O	1:A:587:ILE:HD13	2.18	0.42
1:A:623:PHE:CD2	1:A:639:LEU:HD13	2.54	0.42
1:A:1436:ARG:HB2	1:A:1485:GLY:HA2	2.02	0.42
1:A:1439:ILE:HD12	1:A:1450:ARG:HG3	2.01	0.42
1:A:1722:GLY:H	1:A:1766:GLN:CG	2.33	0.42
1:A:2120:ARG:HG3	1:A:2237:MET:SD	2.59	0.42
1:A:2438:GLN:CG	1:A:2494:LEU:HD21	2.49	0.42
1:B:350:MET:HE2	1:B:350:MET:HB2	1.38	0.42
1:B:387:SER:N	1:B:399:ASN:HD22	2.17	0.42
1:B:1415:TYR:CE2	1:B:1468:VAL:HG21	2.54	0.42
1:B:2304:CYS:SG	1:B:2341:LEU:HD12	2.60	0.42
1:C:27:TYR:HD2	1:C:28:LEU:HD22	1.84	0.42
1:C:111:SER:HA	1:C:1980:LEU:O	2.20	0.42
1:C:332:ILE:CG2	1:C:334:ARG:HD2	2.49	0.42
1:C:339:ASP:CG	1:C:343:ASN:HB2	2.44	0.42
1:C:1058:GLU:HA	1:C:1061:GLU:HG3	2.01	0.42
1:C:1629:GLN:O	1:C:1633:ARG:HG2	2.18	0.42
1:D:192:ARG:NH1	1:D:265:GLN:HG2	2.33	0.42
1:D:1122:TRP:HD1	1:D:1146:ILE:HD11	1.85	0.42
1:D:1334:GLU:CD	1:D:1335:ASN:HB2	2.45	0.42
1:D:1897:ARG:HD3	1:D:1916:TRP:CZ2	2.54	0.42
1:E:33:LEU:HD21	1:E:49:LEU:HD11	2.01	0.42
1:E:324:GLU:O	1:E:351:TYR:CZ	2.72	0.42
1:E:1083:ARG:HH11	1:E:1083:ARG:HG3	1.84	0.42
1:E:1089:ASP:OD2	1:E:1114:ARG:HB3	2.19	0.42
1:E:1633:ARG:HB2	1:E:1641:ILE:HD13	2.01	0.42
1:A:346:TYR:HE1	1:A:360:ARG:HD3	1.83	0.42
1:A:828:LEU:HD12	1:A:831:LEU:HD23	2.02	0.42
1:A:1373:LYS:HA	1:A:1373:LYS:HD2	1.64	0.42
1:A:2389:PHE:CD1	1:A:2395:GLY:HA3	2.54	0.42
1:B:750:ASN:OD1	1:B:753:GLU:HB2	2.20	0.42
1:B:1331:THR:HG22	1:B:1332:VAL:N	2.34	0.42
1:B:1514:ILE:HG13	1:B:1573:THR:HG22	2.01	0.42
1:B:1894:LEU:HD13	1:B:1894:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:GLN:N	1:C:806:THR:HG21	2.34	0.42
1:C:1241:LEU:HB2	1:C:1267:ILE:CG2	2.46	0.42
1:C:1631:VAL:HG12	1:D:1164:GLU:OE2	2.19	0.42
1:C:2030:MET:HE2	1:D:2273:GLN:HE21	1.85	0.42
1:C:2191:ALA:O	1:C:2195:VAL:HG13	2.19	0.42
1:D:169:LEU:HD23	1:D:169:LEU:HA	1.76	0.42
1:D:1856:GLU:HA	1:D:1856:GLU:OE2	2.20	0.42
1:D:2097:GLN:HB3	1:E:2257:TYR:HD1	1.84	0.42
1:E:175:ARG:HB3	1:E:175:ARG:CZ	2.50	0.42
1:E:276:PHE:CD2	1:E:281:TRP:HZ3	2.35	0.42
1:E:373:LEU:HD23	1:E:379:PRO:HA	2.01	0.42
1:E:1415:TYR:CE1	1:E:1417:LYS:HA	2.55	0.42
1:E:1509:ILE:N	1:E:1576:LYS:HE3	2.35	0.42
1:E:1626:LEU:HD13	1:E:1792:MET:HE1	2.01	0.42
1:E:1758:ALA:HB3	1:E:1760:HIS:NE2	2.35	0.42
1:E:1934:GLN:CD	1:E:1934:GLN:N	2.77	0.42
1:E:2436:LEU:CD1	1:E:2501:VAL:HA	2.49	0.42
1:A:404:ILE:HA	1:A:408:GLU:OE1	2.20	0.42
1:A:409:TYR:O	1:A:436:PHE:HB3	2.20	0.42
1:A:851:MET:HE1	1:B:567:ASN:OD1	2.20	0.42
1:A:1095:ALA:HA	1:A:1108:TRP:O	2.20	0.42
1:A:1998:LEU:HD11	1:A:2002:ARG:HH12	1.85	0.42
1:A:2111:ALA:O	1:A:2115:VAL:HG23	2.19	0.42
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.78	0.42
1:B:684:ARG:HG2	1:B:745:LEU:HD13	2.02	0.42
1:B:816:TRP:O	1:B:820:LEU:HG	2.19	0.42
1:B:953:ASN:HB3	1:B:954:ILE:HD12	2.02	0.42
1:B:1281:LEU:HD12	1:B:1281:LEU:HA	1.79	0.42
1:C:126:ALA:HB2	1:C:997:ILE:HD11	2.01	0.42
1:C:1365:GLY:HA3	1:C:1371:ARG:HB3	2.02	0.42
1:C:1642:LEU:HB2	1:C:1832:TYR:HD2	1.85	0.42
1:C:2372:TYR:HD2	1:C:2382:LEU:HD13	1.85	0.42
1:D:190:THR:O	1:D:190:THR:HG22	2.20	0.42
1:D:783:VAL:HG22	1:D:832:ARG:HH21	1.85	0.42
1:D:870:ILE:O	1:D:874:LEU:HG	2.19	0.42
1:D:1451:LEU:HD12	1:D:1479:CYS:SG	2.60	0.42
1:D:1610:ALA:HB2	1:D:1652:PRO:HG2	2.01	0.42
1:D:1902:TYR:CE2	1:D:2007:ILE:HB	2.54	0.42
1:D:1957:LEU:HD23	1:D:1957:LEU:HA	1.77	0.42
1:D:2026:LEU:HD21	1:E:818:ASN:CB	2.49	0.42
1:D:2120:ARG:CA	1:D:2237:MET:HE3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2297:PHE:HA	1:D:2300:THR:HG22	2.01	0.42
1:D:2423:PHE:HE2	1:D:2502:ASN:HB2	1.85	0.42
1:E:28:LEU:HD11	1:E:33:LEU:HA	2.01	0.42
1:E:386:LEU:HA	1:E:399:ASN:CB	2.50	0.42
1:E:1659:PHE:CE1	1:E:1710:PHE:HB2	2.55	0.42
1:E:1967:LYS:HG3	1:E:1968:ASN:H	1.83	0.42
1:E:2057:THR:O	1:E:2061:VAL:HG22	2.19	0.42
1:E:2130:TYR:CD1	1:E:2226:GLN:NE2	2.87	0.42
1:E:2387:THR:HA	1:E:2390:LEU:HD12	2.01	0.42
1:A:160:SER:HB3	1:A:982:LYS:NZ	2.28	0.42
1:A:1358:ALA:HB2	1:A:1547:THR:HG23	2.01	0.42
1:A:1389:TYR:HA	1:A:1541:PHE:CZ	2.55	0.42
1:A:1991:TRP:HB3	1:A:1995:ARG:NH1	2.34	0.42
1:A:2138:ILE:HD13	1:A:2216:TYR:HD2	1.85	0.42
1:A:2395:GLY:O	1:A:2405:LYS:HA	2.19	0.42
1:B:346:TYR:CD2	1:B:360:ARG:CZ	3.03	0.42
1:B:737:ILE:O	1:B:740:PHE:HB3	2.20	0.42
1:B:972:LEU:HD12	1:B:992:GLY:O	2.20	0.42
1:B:1150:VAL:HG13	1:B:1170:TRP:NE1	2.35	0.42
1:B:1627:ALA:O	1:B:1631:VAL:HG23	2.20	0.42
1:B:1853:ARG:N	1:B:1854:PRO:HD2	2.35	0.42
1:B:2090:GLN:HA	1:B:2093:GLU:CD	2.44	0.42
1:B:2328:TRP:CE3	1:B:2334:GLY:HA3	2.55	0.42
1:C:223:ASN:O	1:C:226:VAL:HG22	2.20	0.42
1:C:293:VAL:HA	1:C:296:TYR:CD2	2.54	0.42
1:C:824:GLY:O	1:C:827:THR:HB	2.20	0.42
1:C:1392:ALA:H	1:C:1418:THR:HG23	1.82	0.42
1:C:1902:TYR:CE2	1:C:2007:ILE:HB	2.50	0.42
1:C:1902:TYR:CD2	1:C:2007:ILE:HD13	2.55	0.42
1:C:2002:ARG:HD3	1:D:977:VAL:HG12	2.01	0.42
1:D:352:GLU:HB3	1:D:357:PHE:HZ	1.84	0.42
1:D:416:TYR:HA	1:D:431:GLY:HA2	2.01	0.42
1:D:1197:LEU:HB2	1:D:1203:TRP:CH2	2.55	0.42
1:D:2046:SER:HB3	1:D:2306:MET:HG2	2.01	0.42
1:D:2090:GLN:O	1:D:2093:GLU:HG2	2.19	0.42
1:D:2350:LYS:HE3	1:D:2350:LYS:HB3	1.94	0.42
1:E:4:THR:O	1:E:8:LEU:HD13	2.19	0.42
1:E:245:GLU:O	1:E:249:ILE:HG12	2.20	0.42
1:E:2477:GLY:H	1:E:2480:ASP:HB2	1.83	0.42
1:A:673:SER:OG	1:A:676:ILE:HG12	2.20	0.42
1:A:743:LEU:HD13	1:A:753:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ASN:C	1:A:1117:LEU:HD22	2.45	0.42
1:B:27:TYR:HB3	1:B:28:LEU:CD2	2.50	0.42
1:B:1200:ASP:O	1:B:1200:ASP:OD2	2.37	0.42
1:B:1255:PHE:CD2	1:B:1285:SER:HA	2.54	0.42
1:B:2239:ALA:O	1:B:2242:GLU:HG3	2.19	0.42
1:C:532:LEU:HD12	1:C:532:LEU:H	1.85	0.42
1:C:1092:VAL:HG21	1:C:1109:PHE:CD1	2.47	0.42
1:D:286:TYR:CZ	1:D:452:ILE:HG21	2.55	0.42
1:D:455:CYS:HB2	1:D:460:LEU:O	2.20	0.42
1:D:606:VAL:HG23	1:D:607:HIS:ND1	2.35	0.42
1:D:840:ARG:HD2	1:D:840:ARG:HA	1.79	0.42
1:D:1318:SER:HB2	1:D:1339:PRO:HA	2.02	0.42
1:D:1450:ARG:HD3	1:D:1452:PHE:C	2.45	0.42
1:E:51:HIS:O	1:E:55:GLU:OE1	2.38	0.42
1:E:1281:LEU:HD12	1:E:1281:LEU:HA	1.87	0.42
1:E:2019:GLU:HG2	1:E:2020:PRO:HD2	2.02	0.42
1:E:2416:ARG:HB3	1:E:2419:ASP:HB2	2.02	0.42
1:A:649:TRP:HD1	1:A:812:ARG:HH12	1.68	0.42
1:A:792:LEU:HD12	1:A:867:TRP:CD1	2.55	0.42
1:A:1176:VAL:HG21	1:A:1189:ARG:HD2	2.01	0.42
1:A:1378:MET:HE1	1:A:1393:PHE:CE2	2.55	0.42
1:A:2390:LEU:HD13	1:A:2523:GLU:HG2	2.02	0.42
1:B:301:GLN:OE1	1:B:317:THR:HG23	2.19	0.42
1:B:387:SER:HB2	1:B:399:ASN:ND2	2.35	0.42
1:B:601:THR:O	1:B:605:ARG:HG2	2.19	0.42
1:B:887:PRO:O	1:B:890:ILE:HG12	2.20	0.42
1:B:968:TYR:CD1	1:B:974:ASP:HA	2.55	0.42
1:B:2346:ALA:HB1	1:C:2299:LEU:HD23	2.02	0.42
1:C:1122:TRP:HZ3	1:C:1124:ASN:HD22	1.68	0.42
1:C:1932:GLY:CA	1:C:1935:GLN:HE21	2.28	0.42
1:D:792:LEU:HD12	1:D:867:TRP:CD1	2.55	0.42
1:D:950:PHE:CD2	1:D:967:LEU:HD11	2.54	0.42
1:D:1122:TRP:HZ3	1:D:1124:ASN:ND2	2.18	0.42
1:D:1422:ILE:HB	1:D:1466:PHE:HB2	2.01	0.42
1:D:2157:LEU:HD23	1:D:2157:LEU:O	2.20	0.42
1:E:1182:ASP:HB3	1:E:1183:PRO:HD3	2.01	0.42
1:E:1882:TYR:O	1:E:1886:THR:HG23	2.19	0.42
1:A:51:HIS:O	1:A:54:ILE:HG12	2.20	0.41
1:A:276:PHE:HA	1:A:281:TRP:CE3	2.54	0.41
1:A:1439:ILE:HG13	1:A:1486:ASN:CB	2.50	0.41
1:C:374:ARG:HB3	1:C:375:LYS:H	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:HA	1:C:399:ASN:CB	2.50	0.41
1:C:689:GLU:HA	1:C:692:ALA:HB3	2.02	0.41
1:C:708:ILE:O	1:C:712:LEU:CB	2.67	0.41
1:C:775:ARG:HA	1:C:775:ARG:HD3	1.80	0.41
1:C:948:ASN:C	1:C:948:ASN:HD22	2.28	0.41
1:C:1235:PHE:CD1	1:C:1309:PHE:HD2	2.37	0.41
1:C:1662:PHE:CZ	1:C:1725:LEU:HD13	2.52	0.41
1:C:2339:GLU:HB3	1:D:2292:ILE:HD13	2.02	0.41
1:D:567:ASN:OD1	1:D:568:SER:N	2.52	0.41
1:D:1235:PHE:CE1	1:D:1237:GLY:HA3	2.56	0.41
1:D:1416:ASN:O	1:D:1420:ASN:CA	2.64	0.41
1:D:1878:ASP:CG	1:D:1881:HIS:HD2	2.28	0.41
1:E:236:LEU:HB2	1:E:487:PHE:CD1	2.55	0.41
1:E:310:ALA:HB2	1:E:317:THR:HB	2.02	0.41
1:E:719:MET:HG3	1:E:778:GLU:HG2	2.02	0.41
1:E:1173:LYS:NZ	1:E:1175:GLU:HB3	2.34	0.41
1:E:1409:GLY:HA3	1:E:1427:GLY:H	1.85	0.41
1:E:1437:ARG:O	1:E:1439:ILE:HG12	2.20	0.41
1:E:2164:ILE:HD13	1:E:2164:ILE:HA	1.94	0.41
1:E:2522:LEU:O	1:E:2525:LEU:HB3	2.20	0.41
1:A:226:VAL:HG12	1:A:876:TRP:NE1	2.35	0.41
1:A:1659:PHE:CE1	1:A:1710:PHE:HB2	2.54	0.41
1:A:1915:MET:O	1:A:1918:VAL:HG12	2.20	0.41
1:A:2185:TRP:CZ3	1:D:1174:GLU:HG2	2.55	0.41
1:A:2262:GLN:O	1:A:2265:THR:HG22	2.20	0.41
1:A:2364:ARG:HH11	1:A:2422:ILE:HG12	1.85	0.41
1:B:76:SER:HB3	1:B:80:ARG:NE	2.32	0.41
1:B:732:PRO:HD2	1:B:760:PHE:HE1	1.85	0.41
1:B:1771:LYS:HD3	1:B:1771:LYS:HA	1.83	0.41
1:B:2125:ASN:C	1:B:2129:LYS:HZ2	2.27	0.41
1:C:274:GLU:HG3	1:C:1405:TYR:OH	2.20	0.41
1:C:489:THR:CG2	1:C:507:ASN:HD22	2.33	0.41
1:C:1021:TRP:CZ3	1:C:1025:ASN:HA	2.55	0.41
1:C:1116:ASN:HD22	1:D:1207:TRP:HA	1.85	0.41
1:C:1313:PHE:HE2	1:C:1345:TYR:CE1	2.38	0.41
1:C:1821:LYS:HA	1:C:1821:LYS:HD2	1.75	0.41
1:C:2385:LYS:HD2	1:C:2389:PHE:CZ	2.55	0.41
1:D:192:ARG:HD2	1:D:265:GLN:O	2.19	0.41
1:D:1576:LYS:HB3	1:D:1576:LYS:HE2	1.81	0.41
1:D:2239:ALA:O	1:D:2242:GLU:HG3	2.20	0.41
1:D:2436:LEU:HA	1:D:2534:TYR:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:GLN:HB3	1:E:477:ILE:HG23	2.02	0.41
1:E:623:PHE:HA	1:E:626:LYS:NZ	2.35	0.41
1:E:1050:ILE:HD13	1:E:1870:ASP:OD1	2.19	0.41
1:E:1584:ILE:HD13	1:E:1584:ILE:HA	1.82	0.41
1:E:2474:LEU:HD21	1:E:2477:GLY:CA	2.50	0.41
1:A:216:THR:CG2	1:A:494:HIS:HB3	2.50	0.41
1:A:356:GLN:O	1:A:402:SER:HA	2.20	0.41
1:A:1291:PHE:O	1:A:1293:ILE:HG23	2.20	0.41
1:A:2049:ARG:NH2	1:A:2494:LEU:H	2.19	0.41
1:A:2104:ARG:HD3	1:A:2104:ARG:HA	1.90	0.41
1:B:1649:LEU:CD1	1:B:1650:PRO:HD2	2.48	0.41
1:B:1658:PHE:HZ	1:B:1743:PHE:HD2	1.67	0.41
1:B:1823:PHE:CD2	1:B:1897:ARG:HD3	2.55	0.41
1:B:2000:ASN:OD1	1:B:2005:LEU:HB2	2.20	0.41
1:B:2099:ILE:CD1	1:B:2258:GLN:HB3	2.49	0.41
1:B:2387:THR:O	1:B:2391:ARG:HG3	2.21	0.41
1:B:2438:GLN:HB2	1:B:2494:LEU:HD21	2.02	0.41
1:B:2457:LEU:HD11	1:B:2509:LEU:HG	2.02	0.41
1:C:79:ILE:HB	1:C:1887:PHE:CE2	2.55	0.41
1:C:249:ILE:HA	1:C:252:GLU:OE2	2.19	0.41
1:C:1422:ILE:HB	1:C:1468:VAL:HG22	2.03	0.41
1:C:1508:GLY:HA3	1:C:1576:LYS:HE3	2.02	0.41
1:D:249:ILE:O	1:D:252:GLU:HG2	2.20	0.41
1:D:1166:LEU:HD23	1:D:1167:HIS:N	2.35	0.41
1:D:1487:ASN:N	1:D:1489:GLN:HE22	2.14	0.41
1:D:1523:LYS:NZ	1:D:1557:SER:H	2.18	0.41
1:D:2019:GLU:HG2	1:D:2020:PRO:HD2	2.02	0.41
1:D:2400:SER:C	1:D:2416:ARG:HH21	2.28	0.41
1:E:806:THR:O	1:E:810:LEU:HG	2.19	0.41
1:E:1046:PRO:HG2	1:E:1889:ARG:NH1	2.32	0.41
1:E:1079:THR:O	1:E:1083:ARG:HG2	2.20	0.41
1:E:2138:ILE:HG23	1:E:2142:GLU:HB2	2.02	0.41
1:E:2395:GLY:O	1:E:2405:LYS:HA	2.20	0.41
1:A:22:LEU:HD21	1:A:52:GLU:C	2.45	0.41
1:A:227:MET:HE2	1:A:227:MET:HA	2.01	0.41
1:A:712:LEU:HD21	1:A:768:SER:HB3	2.01	0.41
1:A:854:GLN:HA	1:A:857:VAL:HG22	2.02	0.41
1:A:1399:VAL:C	1:A:1400:LYS:HD3	2.46	0.41
1:A:1823:PHE:HB3	1:A:1897:ARG:CZ	2.50	0.41
1:A:1941:LEU:HD12	1:A:1941:LEU:HA	1.87	0.41
1:A:2184:ARG:CZ	1:E:2184:ARG:HH22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HD21	1:B:1018:PHE:CZ	2.52	0.41
1:B:199:TYR:CD1	1:B:945:VAL:HG21	2.55	0.41
1:B:311:TYR:HB3	1:B:312:VAL:H	1.73	0.41
1:B:323:ASN:HB2	1:B:353:GLY:O	2.20	0.41
1:B:780:GLU:HG2	1:B:781:LEU:N	2.35	0.41
1:B:813:PHE:HD1	1:B:867:TRP:CE3	2.38	0.41
1:B:899:VAL:HG21	1:B:904:LYS:N	2.34	0.41
1:B:1813:CYS:HB2	1:B:1829:TRP:NE1	2.35	0.41
1:C:73:PRO:HA	1:C:80:ARG:NH2	2.35	0.41
1:C:374:ARG:HE	1:C:383:VAL:HG21	1.85	0.41
1:C:833:GLN:HG2	1:C:835:THR:HG22	2.01	0.41
1:C:1158:ARG:HG3	1:C:1159:PRO:HD2	2.01	0.41
1:C:1370:ILE:O	1:C:1374:GLN:HB2	2.20	0.41
1:D:704:LEU:O	1:D:708:ILE:HG12	2.20	0.41
1:D:968:TYR:CD1	1:D:974:ASP:HA	2.56	0.41
1:D:1158:ARG:HG3	1:D:1159:PRO:HD2	2.02	0.41
1:D:1197:LEU:HD23	1:D:1198:ARG:O	2.21	0.41
1:D:2088:LEU:HB3	1:D:2269:LEU:HD12	2.02	0.41
1:D:2251:ALA:O	1:D:2255:VAL:HG23	2.20	0.41
1:D:2530:LEU:HB3	1:D:2532:ILE:CD1	2.50	0.41
1:E:315:ILE:HG22	1:E:316:SER:N	2.36	0.41
1:E:659:ALA:O	1:E:663:LEU:HG	2.21	0.41
1:E:1106:LEU:HD12	1:E:1125:VAL:O	2.20	0.41
1:E:1390:GLY:HA2	1:E:1507:THR:C	2.45	0.41
1:E:1476:PHE:HA	1:E:1479:CYS:SG	2.60	0.41
1:A:62:LEU:HD11	1:A:1865:PRO:HG2	2.03	0.41
1:A:1302:VAL:HG11	1:A:1604:ARG:NH1	2.36	0.41
1:A:2369:ALA:HA	1:A:2382:LEU:HG	2.02	0.41
1:B:165:SER:O	1:B:169:LEU:HD23	2.21	0.41
1:B:577:LEU:HD13	1:B:615:CYS:SG	2.61	0.41
1:B:897:ARG:H	1:B:908:ASN:HB2	1.85	0.41
1:B:1153:TYR:CE1	1:B:1154:LYS:HG3	2.55	0.41
1:B:1317:ALA:O	1:B:1341:ILE:HG12	2.20	0.41
1:B:1374:GLN:O	1:B:1378:MET:HG2	2.20	0.41
1:B:1387:SER:O	1:B:1388:GLN:HG2	2.20	0.41
1:B:2027:LEU:HD23	1:B:2027:LEU:H	1.84	0.41
1:B:2184:ARG:CG	1:B:2187:ALA:HB2	2.50	0.41
1:C:1026:ARG:CZ	1:C:1029:THR:HG21	2.50	0.41
1:C:1074:GLU:CG	1:C:1638:ILE:HD11	2.51	0.41
1:D:77:GLY:N	1:D:1925:GLY:HA3	2.26	0.41
1:D:191:TYR:O	1:D:198:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:PHE:HD1	1:D:563:GLY:HA3	1.83	0.41
1:D:700:GLN:HA	1:D:703:ILE:HG12	2.03	0.41
1:D:817:ILE:HG13	1:D:818:ASN:N	2.35	0.41
1:D:828:LEU:HD12	1:D:831:LEU:HD23	2.03	0.41
1:D:1399:VAL:HG13	1:D:1497:TYR:HB3	2.03	0.41
1:D:1927:GLU:HB3	1:D:1991:TRP:CE2	2.56	0.41
1:D:2436:LEU:HA	1:D:2534:TYR:HB3	2.02	0.41
1:E:23:ALA:HB3	1:E:1955:GLN:OE1	2.21	0.41
1:E:357:PHE:HB2	1:E:400:TYR:HA	2.02	0.41
1:E:359:ILE:HG21	1:E:359:ILE:HD13	1.79	0.41
1:E:498:LEU:HD22	1:E:502:ASP:OD2	2.21	0.41
1:E:971:PHE:O	1:E:973:ILE:HG22	2.21	0.41
1:E:1122:TRP:HZ3	1:E:1124:ASN:ND2	2.18	0.41
1:E:2047:LEU:HD12	1:E:2047:LEU:HA	1.80	0.41
1:A:309:SER:HA	1:A:311:TYR:CE2	2.56	0.41
1:A:336:LYS:HD3	1:A:415:ILE:HG22	2.01	0.41
1:A:1727:VAL:O	1:A:1733:THR:HG23	2.20	0.41
1:B:346:TYR:CD1	1:B:360:ARG:HA	2.56	0.41
1:B:475:GLN:HB2	1:B:477:ILE:HG12	2.03	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.92	0.41
1:B:759:GLN:O	1:B:763:VAL:HG13	2.19	0.41
1:B:1415:TYR:HE1	1:B:1417:LYS:HA	1.85	0.41
1:B:1439:ILE:HD12	1:B:1450:ARG:HG3	2.01	0.41
1:B:1572:GLU:OE2	1:B:1574:LYS:HB3	2.21	0.41
1:B:2054:LEU:HD21	1:B:2058:ARG:HH22	1.85	0.41
1:B:2444:PRO:HD2	1:B:2527:ASP:O	2.19	0.41
1:C:985:ARG:O	1:C:988:GLU:HG3	2.19	0.41
1:C:1074:GLU:HG2	1:C:1638:ILE:HD11	2.02	0.41
1:C:1732:ILE:HD12	1:C:1732:ILE:HA	1.94	0.41
1:D:279:GLN:O	1:D:282:ILE:HG22	2.20	0.41
1:D:352:GLU:N	1:D:357:PHE:CZ	2.89	0.41
1:D:1435:THR:O	1:D:1437:ARG:HG3	2.21	0.41
1:E:349:LEU:HD23	1:E:349:LEU:HA	1.85	0.41
1:E:496:TYR:HD2	1:E:606:VAL:HG22	1.86	0.41
1:E:664:CYS:SG	1:E:803:ASN:HA	2.60	0.41
1:E:2116:LEU:O	1:E:2119:SER:HB2	2.21	0.41
1:E:2353:LEU:HA	1:E:2353:LEU:HD23	1.77	0.41
1:A:289:GLU:O	1:A:292:GLU:HG3	2.20	0.41
1:A:587:ILE:CG1	1:A:593:VAL:HG21	2.48	0.41
1:A:1041:GLU:OE2	1:A:1881:HIS:HD2	2.04	0.41
1:A:1399:VAL:HG13	1:A:1497:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:GLY:HA3	1:A:1427:GLY:HA3	2.02	0.41
1:B:181:SER:O	1:B:185:MET:HG2	2.21	0.41
1:B:1140:TRP:CE2	1:B:1797:ALA:HB2	2.55	0.41
1:B:1177:ALA:HB3	1:C:2176:PHE:CD1	2.56	0.41
1:B:1215:VAL:O	1:B:1219:THR:HG23	2.21	0.41
1:B:1413:THR:OG1	1:B:1422:ILE:HG23	2.20	0.41
1:C:142:ARG:HE	1:C:142:ARG:HB3	1.71	0.41
1:C:173:ILE:HD12	1:C:949:TRP:CZ3	2.56	0.41
1:C:387:SER:H	1:C:399:ASN:CB	2.31	0.41
1:C:416:TYR:HA	1:C:431:GLY:HA2	2.02	0.41
1:C:1378:MET:HE1	1:C:1393:PHE:CG	2.56	0.41
1:C:1624:THR:O	1:C:1625:LEU:HD23	2.20	0.41
1:C:1633:ARG:HB3	1:C:1640:THR:HG22	2.02	0.41
1:C:2315:LEU:HD21	1:C:2355:ARG:CZ	2.50	0.41
1:D:25:LEU:C	1:D:27:TYR:HB2	2.45	0.41
1:D:780:GLU:HG3	1:D:817:ILE:HD13	2.02	0.41
1:D:1235:PHE:HB3	1:D:1240:THR:HG22	2.02	0.41
1:D:1748:THR:HG23	1:D:1749:LYS:HD2	2.02	0.41
1:D:1845:ILE:HD11	1:E:1003:ARG:HH21	1.84	0.41
1:E:464:GLU:OE2	1:E:500:PHE:HB2	2.21	0.41
1:E:1537:PRO:HG3	1:E:1546:TYR:CE2	2.55	0.41
1:E:2120:ARG:HD2	1:E:2238:ASP:OD1	2.20	0.41
1:A:14:THR:HG23	1:A:16:ASP:H	1.85	0.41
1:A:330:TYR:HD2	1:A:436:PHE:HE2	1.69	0.41
1:A:603:LEU:HG	1:A:614:LEU:HD11	2.02	0.41
1:A:705:ALA:N	1:A:706:PRO:HD2	2.36	0.41
1:A:883:LEU:O	1:A:885:THR:HG23	2.20	0.41
1:A:1415:TYR:CD1	1:A:1417:LYS:HG2	2.56	0.41
1:A:1746:ASP:OD1	1:A:1748:THR:HG22	2.21	0.41
1:A:2415:VAL:CG1	1:A:2420:LEU:HD21	2.50	0.41
1:B:172:HIS:HA	1:B:175:ARG:HH11	1.86	0.41
1:B:774:LEU:HB3	1:B:776:LEU:CD2	2.51	0.41
1:B:1438:LEU:HG	1:B:1466:PHE:CE2	2.56	0.41
1:B:1516:ILE:HD11	1:B:1569:ILE:CG2	2.51	0.41
1:B:1970:ARG:HD2	1:B:1970:ARG:HA	1.97	0.41
1:B:2337:ALA:O	1:B:2341:LEU:HD23	2.21	0.41
1:C:416:TYR:CD1	1:C:431:GLY:HA3	2.51	0.41
1:C:946:LEU:HD23	1:C:946:LEU:HA	1.87	0.41
1:C:1523:LYS:HZ3	1:C:1556:SER:H	1.68	0.41
1:D:1436:ARG:HG3	1:D:1456:PHE:CE2	2.55	0.41
1:D:2513:ASP:OD1	1:D:2516:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:PHE:CE2	1:E:417:ALA:HB3	2.56	0.41
1:E:463:ASN:HA	1:E:466:GLN:CD	2.45	0.41
1:E:2437:LYS:O	1:E:2494:LEU:HD23	2.19	0.41
1:A:185:MET:HE3	1:A:185:MET:HB3	1.96	0.41
1:A:192:ARG:NH1	1:A:265:GLN:HG2	2.36	0.41
1:A:391:ILE:HG12	1:A:396:PHE:CE2	2.55	0.41
1:A:537:PHE:CE1	1:A:555:PHE:CD2	3.09	0.41
1:A:1477:LYS:HZ2	1:A:1502:TRP:HB2	1.86	0.41
1:A:1527:PHE:CD2	1:A:1551:LEU:HD13	2.56	0.41
1:A:1691:ARG:HE	1:A:1691:ARG:HB3	1.68	0.41
1:A:2165:ALA:HA	1:D:1117:LEU:HD11	2.02	0.41
1:B:192:ARG:NH1	1:B:265:GLN:HG2	2.36	0.41
1:B:346:TYR:CE2	1:B:365:VAL:HA	2.54	0.41
1:B:1156:ALA:HB3	1:B:1171:VAL:HG22	2.02	0.41
1:B:1523:LYS:NZ	1:B:1557:SER:H	2.18	0.41
1:B:1527:PHE:CD1	1:B:1532:HIS:CE1	3.09	0.41
1:B:1588:LEU:HD12	1:B:1589:SER:H	1.86	0.41
1:B:2343:LEU:HD12	1:C:2292:ILE:HG23	2.03	0.41
1:C:70:ARG:HH11	1:C:70:ARG:HG3	1.86	0.41
1:C:256:GLU:HG3	1:C:443:ILE:HD11	2.02	0.41
1:C:311:TYR:O	1:C:312:VAL:C	2.64	0.41
1:C:420:TYR:HA	1:C:425:SER:O	2.21	0.41
1:C:470:ARG:NH1	1:C:514:TYR:HE2	2.18	0.41
1:C:1108:TRP:CD1	1:C:1108:TRP:N	2.88	0.41
1:C:1229:ALA:HB3	1:C:1246:TYR:CE2	2.55	0.41
1:C:1410:GLY:N	1:C:1426:GLN:HG3	2.35	0.41
1:C:1414:VAL:O	1:C:1422:ILE:HD12	2.21	0.41
1:C:1414:VAL:HG22	1:C:1415:TYR:H	1.85	0.41
1:C:1825:GLU:HA	1:C:1828:GLN:HG3	2.03	0.41
1:C:1866:LEU:HD23	1:C:1866:LEU:HA	1.81	0.41
1:C:2019:GLU:HG2	1:C:2020:PRO:HD2	2.03	0.41
1:C:2116:LEU:HD23	1:C:2116:LEU:HA	1.84	0.41
1:C:2174:ASN:HA	1:D:2185:TRP:HE1	1.86	0.41
1:C:2368:LEU:HD13	1:C:2368:LEU:HA	1.95	0.41
1:C:2419:ASP:O	1:C:2421:LYS:HG3	2.21	0.41
1:D:192:ARG:HD2	1:D:265:GLN:HG2	2.03	0.41
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.56	0.41
1:D:273:PRO:HG2	1:D:442:THR:HG22	2.02	0.41
1:D:292:GLU:OE1	1:D:296:TYR:HE2	2.04	0.41
1:D:495:ARG:HD2	1:D:644:TYR:CE2	2.56	0.41
1:D:642:TRP:O	1:D:645:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:ALA:N	1:D:706:PRO:HD2	2.36	0.41
1:D:873:VAL:O	1:D:877:ILE:HG22	2.21	0.41
1:D:919:ALA:O	1:D:922:MET:HG3	2.20	0.41
1:D:1083:ARG:HG3	1:D:1083:ARG:HH11	1.86	0.41
1:D:1116:ASN:HB2	1:E:1207:TRP:CD1	2.55	0.41
1:D:1246:TYR:CD1	1:D:1291:PHE:HE1	2.38	0.41
1:D:1276:MET:SD	1:D:1276:MET:N	2.89	0.41
1:D:1443:VAL:HG13	1:D:1445:ASN:H	1.85	0.41
1:D:1756:ASN:HB2	1:D:1774:LYS:O	2.21	0.41
1:D:2115:VAL:HG22	1:E:2239:ALA:CB	2.49	0.41
1:D:2254:GLN:O	1:D:2257:TYR:HB3	2.21	0.41
1:D:2402:ASN:HA	1:D:2414:SER:O	2.21	0.41
1:E:73:PRO:HA	1:E:80:ARG:NH2	2.35	0.41
1:E:249:ILE:O	1:E:252:GLU:HG2	2.20	0.41
1:E:273:PRO:CG	1:E:442:THR:HG22	2.50	0.41
1:E:347:PHE:HD2	1:E:415:ILE:O	2.04	0.41
1:E:414:LYS:H	1:E:434:PHE:CB	2.33	0.41
1:E:415:ILE:HG23	1:E:415:ILE:HD12	1.81	0.41
1:E:535:LYS:NZ	1:E:536:ILE:HG22	2.36	0.41
1:E:719:MET:CG	1:E:778:GLU:HG2	2.51	0.41
1:E:760:PHE:O	1:E:763:VAL:HG12	2.20	0.41
1:E:777:SER:CB	1:E:2274:ARG:HD2	2.48	0.41
1:E:984:THR:HG23	1:E:987:ALA:H	1.86	0.41
1:E:1248:THR:HG22	1:E:1294:ILE:HG12	2.03	0.41
1:E:1746:ASP:OD2	1:E:1749:LYS:HD3	2.20	0.41
1:E:1991:TRP:HB3	1:E:1995:ARG:NH1	2.33	0.41
1:E:2121:ARG:O	1:E:2124:GLN:HG3	2.21	0.41
1:E:2417:LEU:HD21	1:E:2507:LEU:HB2	2.02	0.41
1:A:136:TYR:HD1	1:A:141:ARG:NH1	2.19	0.41
1:A:158:GLU:HB3	1:A:982:LYS:HB3	2.03	0.41
1:A:215:SER:C	1:A:217:LEU:H	2.28	0.41
1:A:272:THR:HG23	1:A:275:ASN:H	1.86	0.41
1:A:684:ARG:HG2	1:A:745:LEU:HD13	2.01	0.41
1:A:728:ASP:HB2	1:A:737:ILE:HG12	2.02	0.41
1:A:801:GLN:O	1:A:806:THR:HG21	2.21	0.41
1:A:1172:GLU:O	1:A:1190:PHE:HA	2.21	0.41
1:A:1518:VAL:HG21	1:A:1553:ILE:CD1	2.51	0.41
1:A:2088:LEU:HD11	1:A:2272:LEU:HD12	2.02	0.41
1:B:299:MET:HE1	1:B:301:GLN:NE2	2.36	0.41
1:B:321:VAL:HG12	1:B:351:TYR:CE2	2.56	0.41
1:B:478:ILE:HA	1:B:482:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:ALA:O	1:B:902:LEU:HB2	2.21	0.41
1:B:1511:ASN:ND2	1:B:1530:SER:HA	2.36	0.41
1:B:1732:ILE:HD12	1:B:1732:ILE:HA	1.93	0.41
1:B:2142:GLU:HG2	1:B:2216:TYR:CE2	2.39	0.41
1:C:129:LEU:HD11	1:C:1018:PHE:CE2	2.48	0.41
1:C:192:ARG:HD2	1:C:265:GLN:O	2.21	0.41
1:C:462:PRO:O	1:C:465:LEU:HG	2.21	0.41
1:C:740:PHE:O	1:C:744:VAL:HG23	2.20	0.41
1:C:984:THR:HG23	1:C:987:ALA:H	1.86	0.41
1:C:999:ARG:HH21	1:C:1005:GLU:HG2	1.86	0.41
1:C:1195:ALA:HB2	1:C:1206:PRO:HB3	2.02	0.41
1:C:1318:SER:O	1:C:1319:LEU:HD22	2.21	0.41
1:C:1976:VAL:O	1:C:1976:VAL:HG13	2.20	0.41
1:D:890:ILE:O	1:D:894:VAL:HG12	2.21	0.41
1:D:1371:ARG:HG3	1:D:1372:ASN:H	1.86	0.41
1:E:113:PHE:HZ	1:E:1038:TYR:CD2	2.39	0.41
1:E:207:ARG:HH21	1:E:240:ALA:HA	1.86	0.41
1:E:217:LEU:HB3	1:E:220:LEU:CB	2.51	0.41
1:E:566:VAL:HB	1:E:570:GLU:HG2	2.03	0.41
1:E:1056:MET:HE1	1:E:1809:THR:HA	2.03	0.41
1:E:1150:VAL:HG22	1:E:1152:PRO:HD3	2.02	0.41
1:E:1387:SER:O	1:E:1388:GLN:HG2	2.20	0.41
1:E:1518:VAL:HG21	1:E:1553:ILE:CD1	2.51	0.41
1:E:2184:ARG:HG2	1:E:2187:ALA:HB2	2.01	0.41
1:A:816:TRP:CE2	1:A:820:LEU:HD21	2.56	0.40
1:A:1132:ALA:HB1	1:A:1618:TYR:OH	2.21	0.40
1:A:2115:VAL:HG22	1:B:2239:ALA:CB	2.50	0.40
1:A:2328:TRP:CE3	1:A:2334:GLY:HA3	2.56	0.40
1:A:2516:ASP:H	1:A:2519:LYS:CB	2.30	0.40
1:B:51:HIS:O	1:B:55:GLU:OE1	2.38	0.40
1:B:327:LEU:HD12	1:B:327:LEU:O	2.21	0.40
1:B:336:LYS:HA	1:B:432:GLY:HA3	2.03	0.40
1:B:348:ASP:HB2	1:B:359:ILE:HG21	2.03	0.40
1:B:452:ILE:HD12	1:B:455:CYS:SG	2.61	0.40
1:B:2185:TRP:CZ3	1:E:1174:GLU:HG2	2.56	0.40
1:B:2285:MET:O	1:B:2289:LEU:HD23	2.21	0.40
1:C:62:LEU:HD23	1:C:62:LEU:HA	1.87	0.40
1:C:349:LEU:HD11	1:C:404:ILE:HB	2.03	0.40
1:C:1405:TYR:HB2	1:C:1430:MET:CE	2.50	0.40
1:C:2390:LEU:HD21	1:C:2522:LEU:HD23	2.01	0.40
1:D:602:LEU:O	1:D:606:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1106:LEU:HD12	1:D:1125:VAL:O	2.21	0.40
1:D:1265:MET:CA	1:D:1276:MET:HE1	2.51	0.40
1:D:1817:LEU:HD23	1:D:1817:LEU:HA	1.85	0.40
1:D:2050:PHE:CZ	1:D:2054:LEU:HD21	2.56	0.40
1:D:2272:LEU:HG	1:D:2275:LYS:HZ1	1.85	0.40
1:D:2409:ARG:NH1	1:D:2513:ASP:HA	2.37	0.40
1:E:206:ILE:O	1:E:210:ILE:HG12	2.21	0.40
1:E:492:TYR:CE2	1:E:506:LEU:HD22	2.56	0.40
1:E:1059:LEU:HD12	1:E:1080:TYR:CB	2.50	0.40
1:E:1648:ARG:HA	1:E:1853:ARG:NH1	2.36	0.40
1:E:2192:SER:HA	1:E:2195:VAL:HG22	2.03	0.40
1:A:321:VAL:CG1	1:A:352:GLU:HA	2.51	0.40
1:A:2163:SER:HB3	1:A:2195:VAL:HG12	2.03	0.40
1:B:290:LEU:O	1:B:293:VAL:HG22	2.20	0.40
1:B:310:ALA:HB3	1:B:330:TYR:CE2	2.55	0.40
1:B:345:ASN:ND2	1:B:364:LYS:HE3	2.35	0.40
1:B:501:ASP:HB3	1:B:522:HIS:NE2	2.36	0.40
1:B:554:THR:HG22	1:B:556:ALA:H	1.86	0.40
1:B:1162:PHE:CD2	1:B:1163:ARG:HG2	2.56	0.40
1:B:2045:LEU:HD23	1:B:2466:PRO:HD2	2.03	0.40
1:B:2166:GLU:HG3	1:C:2190:ARG:HB2	2.03	0.40
1:C:1255:PHE:CD2	1:C:1285:SER:HA	2.57	0.40
1:C:1395:ILE:HG22	1:C:1414:VAL:CG2	2.51	0.40
1:C:1413:THR:HA	1:C:1424:SER:HA	2.03	0.40
1:C:1713:TYR:HD1	1:C:1718:TYR:OH	2.04	0.40
1:D:323:ASN:HB3	1:D:353:GLY:O	2.21	0.40
1:D:334:ARG:HB2	1:D:433:ILE:O	2.21	0.40
1:D:345:ASN:ND2	1:D:362:ASN:HB2	2.36	0.40
1:D:345:ASN:HD22	1:D:346:TYR:HB2	1.86	0.40
1:D:524:ASN:CG	1:D:528:ASN:HD22	2.29	0.40
1:D:1125:VAL:HG23	1:D:1139:ALA:O	2.21	0.40
1:D:2059:ASN:OD1	1:D:2060:LEU:HD12	2.21	0.40
1:D:2438:GLN:CG	1:D:2494:LEU:HD21	2.52	0.40
1:E:345:ASN:HA	1:E:362:ASN:OD1	2.21	0.40
1:E:364:LYS:HD2	1:E:364:LYS:O	2.21	0.40
1:E:730:LEU:HD23	1:E:730:LEU:HA	1.91	0.40
1:E:1150:VAL:HG23	1:E:1170:TRP:NE1	2.36	0.40
1:E:1175:GLU:O	1:E:1175:GLU:HG2	2.21	0.40
1:E:1666:LYS:HE2	1:E:1703:SER:HA	2.04	0.40
1:E:1713:TYR:CG	1:E:1714:ALA:N	2.88	0.40
1:A:347:PHE:CE1	1:A:417:ALA:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:TRP:HE1	1:A:845:MET:HE1	1.86	0.40
1:A:835:THR:O	1:A:837:THR:HG23	2.21	0.40
1:A:1122:TRP:HZ3	1:A:1124:ASN:ND2	2.20	0.40
1:A:1158:ARG:HG3	1:A:1159:PRO:HD2	2.02	0.40
1:A:2027:LEU:HD23	1:A:2027:LEU:H	1.85	0.40
1:A:2302:SER:O	1:A:2306:MET:HG2	2.21	0.40
1:A:2436:LEU:HB2	1:A:2499:ILE:HB	2.03	0.40
1:B:272:THR:HG23	1:B:274:GLU:HB2	2.03	0.40
1:B:463:ASN:O	1:B:467:THR:HG23	2.22	0.40
1:B:702:GLU:HG2	1:B:721:ARG:HD2	2.04	0.40
1:B:1792:MET:N	1:B:1853:ARG:HH12	2.19	0.40
1:B:1818:LEU:HD12	1:B:1818:LEU:HA	1.79	0.40
1:B:1898:GLY:HA3	1:B:1917:TYR:CE1	2.56	0.40
1:C:602:LEU:O	1:C:606:VAL:HG13	2.21	0.40
1:C:753:GLU:HA	1:C:756:GLN:HG2	2.03	0.40
1:C:1041:GLU:OE2	1:C:1881:HIS:CD2	2.74	0.40
1:D:2219:ARG:HD3	1:D:2223:TRP:CZ2	2.56	0.40
1:E:332:ILE:HG22	1:E:334:ARG:CD	2.50	0.40
1:E:1078:LYS:HD2	1:E:1078:LYS:N	2.36	0.40
1:E:1106:LEU:HD12	1:E:1106:LEU:HA	1.80	0.40
1:E:1292:ASP:OD2	1:E:1301:LEU:HD11	2.21	0.40
1:E:1576:LYS:H	1:E:1576:LYS:HG2	1.70	0.40
1:E:1685:VAL:HB	1:E:1717:TYR:HE1	1.86	0.40
1:E:1902:TYR:CE2	1:E:2007:ILE:HB	2.56	0.40
1:E:2242:GLU:O	1:E:2246:ILE:HG22	2.22	0.40
1:A:480:ASP:HA	1:A:483:LEU:HG	2.03	0.40
1:A:640:VAL:HA	1:A:643:LEU:HG	2.01	0.40
1:A:1084:PHE:HA	1:A:1087:VAL:HG12	2.03	0.40
1:A:1281:LEU:HD12	1:A:1281:LEU:HA	1.82	0.40
1:A:1313:PHE:HA	1:A:1591:LYS:O	2.21	0.40
1:A:2184:ARG:HH22	1:E:2184:ARG:HH22	1.67	0.40
1:A:2438:GLN:HB3	1:A:2533:ARG:HB2	2.03	0.40
1:A:2515:THR:H	1:A:2516:ASP:CG	2.28	0.40
1:B:371:ALA:HA	1:B:382:ILE:HG23	2.03	0.40
1:B:1009:ARG:O	1:B:1012:VAL:HG12	2.21	0.40
1:B:1125:VAL:HG23	1:B:1139:ALA:O	2.21	0.40
1:B:1415:TYR:HB2	1:B:1476:PHE:CE2	2.57	0.40
1:B:1727:VAL:O	1:B:1733:THR:HG23	2.22	0.40
1:B:2202:ALA:HA	1:B:2205:TYR:HD2	1.86	0.40
1:B:2339:GLU:HG3	1:C:2067:PHE:CE1	2.52	0.40
1:C:67:ILE:HD12	1:C:67:ILE:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:SER:HB3	1:C:281:TRP:CB	2.51	0.40
1:C:1527:PHE:CD1	1:C:1532:HIS:CE1	3.10	0.40
1:C:1804:GLU:O	1:C:1809:THR:HG23	2.20	0.40
1:C:1821:LYS:HZ1	1:C:1896:LEU:HD12	1.86	0.40
1:C:2465:MET:HG2	1:C:2466:PRO:CD	2.41	0.40
1:D:224:PRO:HA	1:D:227:MET:SD	2.61	0.40
1:D:330:TYR:HB3	1:D:438:SER:HA	2.04	0.40
1:D:334:ARG:CB	1:D:434:PHE:HA	2.51	0.40
1:D:452:ILE:HA	1:D:455:CYS:SG	2.62	0.40
1:D:885:THR:HG22	1:D:886:MET:N	2.36	0.40
1:D:1236:GLN:O	1:D:1236:GLN:HG3	2.22	0.40
1:D:1664:LEU:HA	1:D:1665:PRO:HD3	1.97	0.40
1:D:2360:LEU:CD1	1:E:2472:ILE:HD12	2.50	0.40
1:E:217:LEU:HB3	1:E:220:LEU:HB3	2.02	0.40
1:E:789:PHE:HB2	1:E:799:ALA:HA	2.03	0.40
1:E:1125:VAL:HG23	1:E:1139:ALA:O	2.21	0.40
1:E:1676:ARG:NH2	1:E:1698:MET:HE3	2.37	0.40
1:A:536:ILE:HD11	1:A:538:GLU:CD	2.46	0.40
1:A:959:VAL:HG12	1:A:961:LEU:H	1.86	0.40
1:A:1265:MET:CA	1:A:1276:MET:HE1	2.52	0.40
1:B:67:ILE:HD12	1:B:67:ILE:HA	1.96	0.40
1:B:73:PRO:HA	1:B:80:ARG:NH2	2.36	0.40
1:B:410:LYS:HD2	1:B:437:GLU:HA	2.04	0.40
1:B:697:ARG:HA	1:B:700:GLN:OE1	2.22	0.40
1:B:1458:PRO:HG2	1:B:1460:THR:O	2.22	0.40
1:B:1601:LEU:HA	1:B:1614:GLN:O	2.22	0.40
1:B:1704:GLU:OE2	1:B:1780:LEU:HD13	2.22	0.40
1:B:2422:ILE:HD12	1:B:2501:VAL:O	2.22	0.40
1:C:840:ARG:HA	1:C:840:ARG:HD2	1.78	0.40
1:C:1190:PHE:CG	1:C:1215:VAL:HG11	2.57	0.40
1:C:1276:MET:HG2	1:C:1281:LEU:HG	2.04	0.40
1:C:1287:LEU:HD23	1:C:1287:LEU:HA	1.73	0.40
1:C:1516:ILE:HD11	1:C:1569:ILE:CG2	2.51	0.40
1:C:1831:ASN:HA	1:C:1834:TYR:O	2.21	0.40
1:C:1870:ASP:OD2	1:C:1872:ASP:HB2	2.21	0.40
1:C:2174:ASN:ND2	1:D:2182:GLY:HA2	2.37	0.40
1:C:2336:MET:HE2	1:D:2288:LYS:NZ	2.37	0.40
1:D:273:PRO:CG	1:D:442:THR:HG22	2.52	0.40
1:D:460:LEU:HD12	1:D:464:GLU:OE1	2.21	0.40
1:D:561:MET:HE3	1:D:568:SER:H	1.87	0.40
1:D:875:GLN:O	1:D:879:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1009:ARG:O	1:D:1012:VAL:HG12	2.22	0.40
1:D:1250:LYS:HE3	1:D:1295:HIS:O	2.21	0.40
1:D:1387:SER:C	1:D:1389:TYR:H	2.29	0.40
1:D:1477:LYS:NZ	1:D:1502:TRP:HB2	2.37	0.40
1:D:2262:GLN:O	1:D:2265:THR:HG22	2.20	0.40
1:E:76:SER:HB3	1:E:80:ARG:NE	2.36	0.40
1:E:336:LYS:O	1:E:339:ASP:HB3	2.22	0.40
1:E:349:LEU:HA	1:E:357:PHE:O	2.22	0.40
1:E:604:ALA:HA	1:E:614:LEU:HD21	2.03	0.40
1:E:739:GLY:O	1:E:742:THR:HG22	2.21	0.40
1:E:1267:ILE:HD12	1:E:1267:ILE:HA	1.95	0.40
1:E:1456:PHE:HZ	1:E:1461:ILE:HD12	1.86	0.40
1:E:1605:GLU:HA	1:E:1611:GLN:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2535/2538 (100%)	2328 (92%)	205 (8%)	2 (0%)	48	80
1	B	2535/2538 (100%)	2329 (92%)	202 (8%)	4 (0%)	43	74
1	C	2535/2538 (100%)	2332 (92%)	199 (8%)	4 (0%)	43	74
1	D	2535/2538 (100%)	2319 (92%)	212 (8%)	4 (0%)	43	74
1	E	2535/2538 (100%)	2329 (92%)	202 (8%)	4 (0%)	43	74
All	All	12675/12690 (100%)	11637 (92%)	1020 (8%)	18 (0%)	49	80

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	ASN

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Mol	Chain	Res	Type
1	B	2516	ASP
1	C	343	ASN
1	C	2516	ASP
1	D	343	ASN
1	D	2516	ASP
1	E	343	ASN
1	E	2516	ASP
1	A	343	ASN
1	C	902	LEU
1	D	902	LEU
1	C	345	ASN
1	A	1730	GLN
1	B	1730	GLN
1	E	1730	GLN
1	B	2137	ASP
1	D	1730	GLN
1	E	344	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2171/2175 (100%)	2171 (100%)	0	100	100
1	B	2172/2175 (100%)	2172 (100%)	0	100	100
1	C	2172/2175 (100%)	2172 (100%)	0	100	100
1	D	2172/2175 (100%)	2172 (100%)	0	100	100
1	E	2172/2175 (100%)	2172 (100%)	0	100	100
All	All	10859/10875 (100%)	10859 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	248	ASN
1	A	302	ASN
1	A	345	ASN
1	A	354	ASN
1	A	362	ASN
1	A	429	GLN
1	A	449	ASN
1	A	512	ASN
1	A	585	ASN
1	A	645	GLN
1	A	962	HIS
1	A	976	GLN
1	A	1103	ASN
1	A	1167	HIS
1	A	1286	GLN
1	A	1311	GLN
1	A	1340	GLN
1	A	1355	HIS
1	A	1489	GLN
1	A	1498	GLN
1	A	1594	ASN
1	A	1635	ASN
1	A	1766	GLN
1	A	1862	ASN
1	A	1864	ASN
1	A	1935	GLN
1	A	1954	GLN
1	A	2063	GLN
1	A	2102	GLN
1	A	2295	GLN
1	A	2308	GLN
1	A	2329	ASN
1	B	265	GLN
1	B	513	GLN
1	B	528	ASN
1	B	573	GLN
1	B	682	ASN
1	B	797	GLN
1	B	868	GLN
1	B	962	HIS
1	B	1103	ASN
1	B	1311	GLN

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Mol	Chain	Res	Type
1	B	1340	GLN
1	B	1349	ASN
1	B	1401	HIS
1	B	1487	ASN
1	B	1532	HIS
1	B	1586	GLN
1	B	1614	GLN
1	B	1635	ASN
1	B	1766	GLN
1	B	1935	GLN
1	B	1954	GLN
1	B	2090	GLN
1	B	2102	GLN
1	B	2258	GLN
1	B	2264	HIS
1	B	2329	ASN
1	B	2402	ASN
1	B	2435	GLN
1	C	60	ASN
1	C	137	HIS
1	C	294	GLN
1	C	302	ASN
1	C	322	ASN
1	C	403	ASN
1	C	449	ASN
1	C	494	HIS
1	C	504	GLN
1	C	585	ASN
1	C	645	GLN
1	C	772	GLN
1	C	822	ASN
1	C	916	GLN
1	C	1002	ASN
1	C	1052	GLN
1	C	1103	ASN
1	C	1167	HIS
1	C	1199	HIS
1	C	1311	GLN
1	C	1340	GLN
1	C	1355	HIS
1	C	1614	GLN
1	C	1862	ASN

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Mol	Chain	Res	Type
1	C	1893	GLN
1	C	1935	GLN
1	C	1954	GLN
1	C	2155	GLN
1	C	2240	GLN
1	C	2329	ASN
1	C	2402	ASN
1	C	2408	ASN
1	D	40	GLN
1	D	60	ASN
1	D	172	HIS
1	D	275	ASN
1	D	302	ASN
1	D	449	ASN
1	D	463	ASN
1	D	466	GLN
1	D	473	ASN
1	D	528	ASN
1	D	682	ASN
1	D	797	GLN
1	D	802	HIS
1	D	814	HIS
1	D	818	ASN
1	D	976	GLN
1	D	998	ASN
1	D	1103	ASN
1	D	1167	HIS
1	D	1311	GLN
1	D	1355	HIS
1	D	1431	ASN
1	D	1489	GLN
1	D	1614	GLN
1	D	1730	GLN
1	D	1862	ASN
1	D	1935	GLN
1	D	1954	GLN
1	D	2155	GLN
1	D	2254	GLN
1	D	2264	HIS
1	D	2295	GLN
1	D	2329	ASN
1	D	2408	ASN

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Mol	Chain	Res	Type
1	D	2502	ASN
1	E	48	HIS
1	E	60	ASN
1	E	200	HIS
1	E	323	ASN
1	E	356	GLN
1	E	449	ASN
1	E	522	HIS
1	E	682	ASN
1	E	713	HIS
1	E	756	GLN
1	E	955	GLN
1	E	1024	ASN
1	E	1052	GLN
1	E	1103	ASN
1	E	1311	GLN
1	E	1335	ASN
1	E	1489	GLN
1	E	1510	ASN
1	E	1611	GLN
1	E	1766	GLN
1	E	1819	GLN
1	E	1822	GLN
1	E	1862	ASN
1	E	1935	GLN
1	E	1954	GLN
1	E	2000	ASN
1	E	2160	GLN
1	E	2264	HIS
1	E	2308	GLN
1	E	2410	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

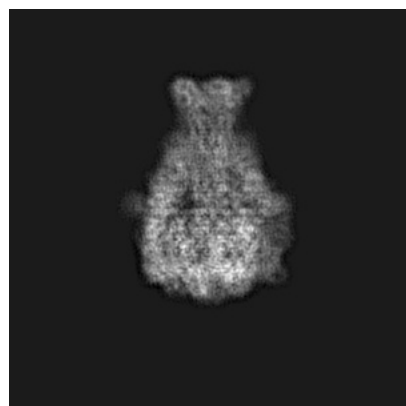
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48372. These allow visual inspection of the internal detail of the map and identification of artifacts.

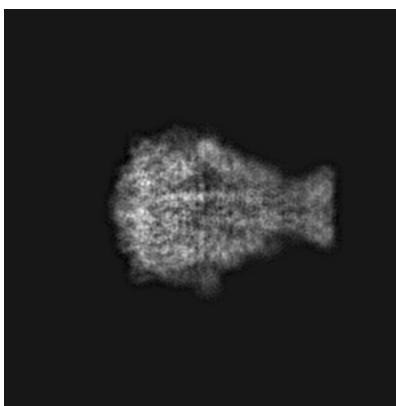
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

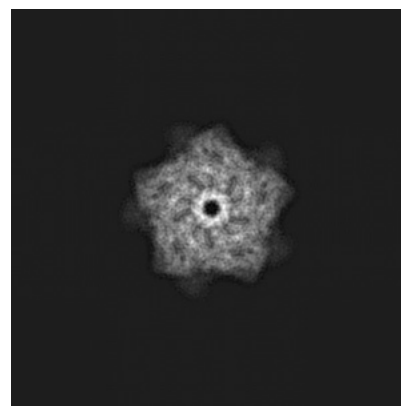
6.1.1 Primary map



X

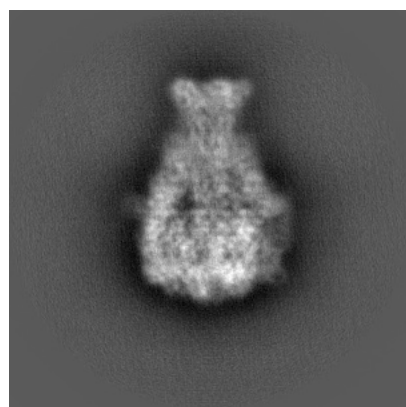


Y

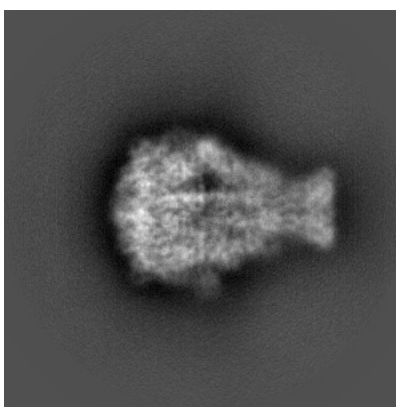


Z

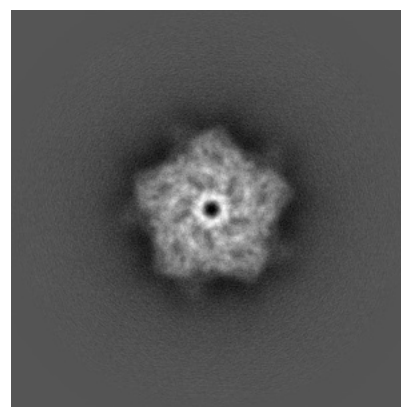
6.1.2 Raw map



X



Y

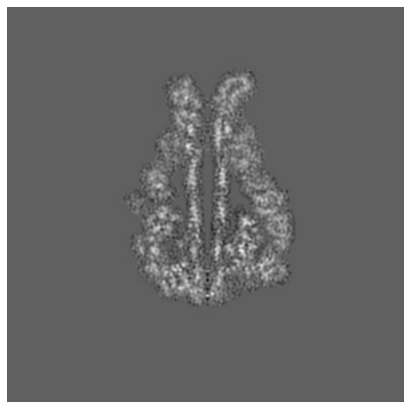


Z

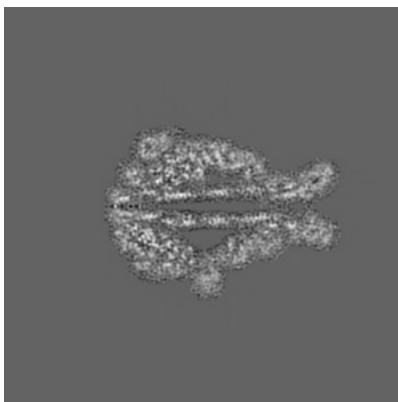
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

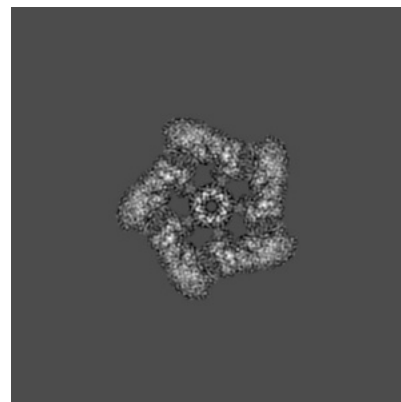
6.2.1 Primary map



X Index: 173

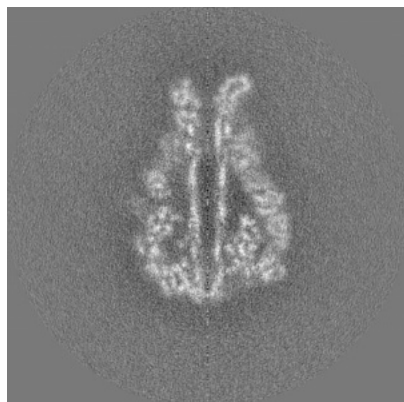


Y Index: 173

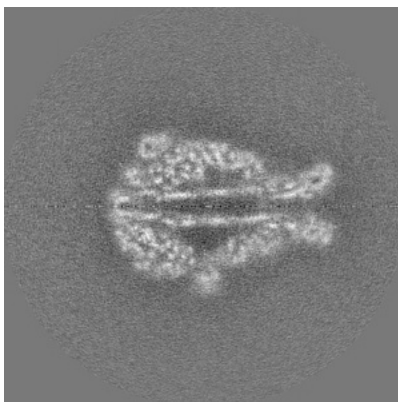


Z Index: 173

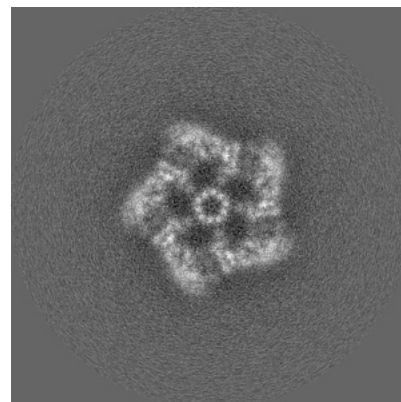
6.2.2 Raw map



X Index: 173



Y Index: 173

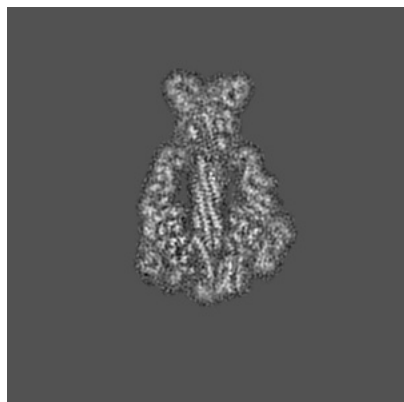


Z Index: 173

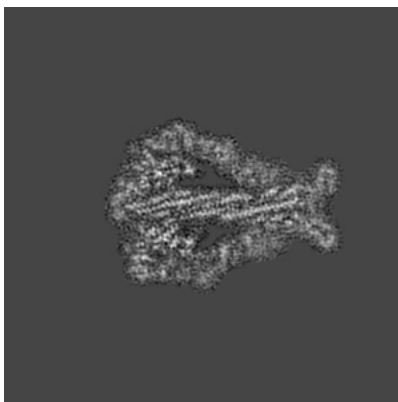
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

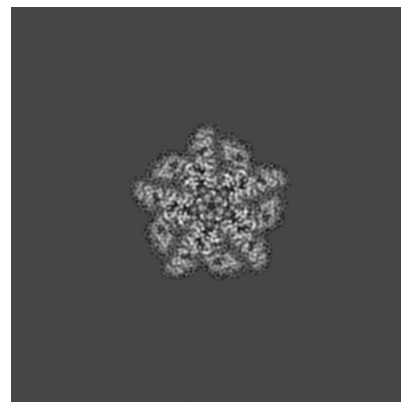
6.3.1 Primary map



X Index: 184

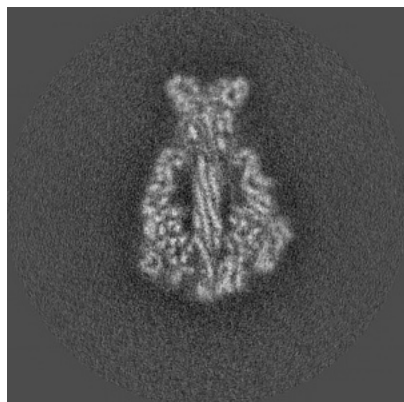


Y Index: 183

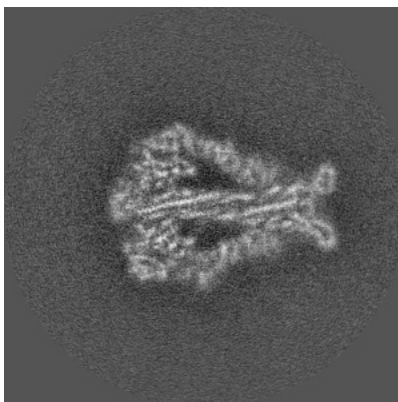


Z Index: 119

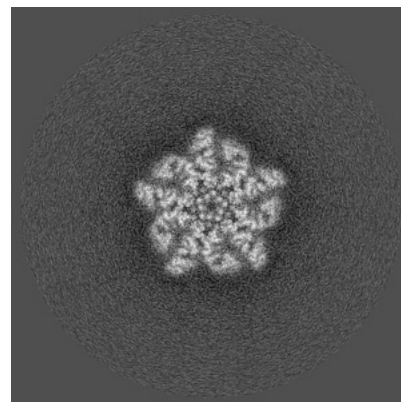
6.3.2 Raw map



X Index: 184



Y Index: 182

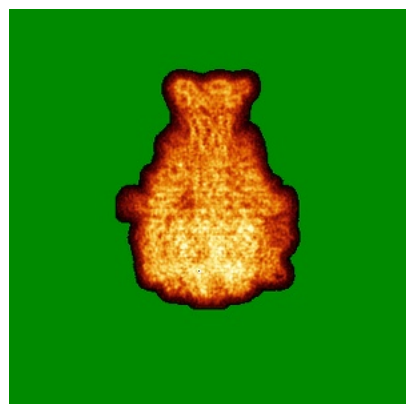


Z Index: 119

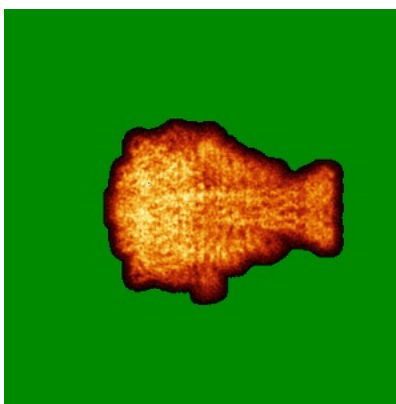
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

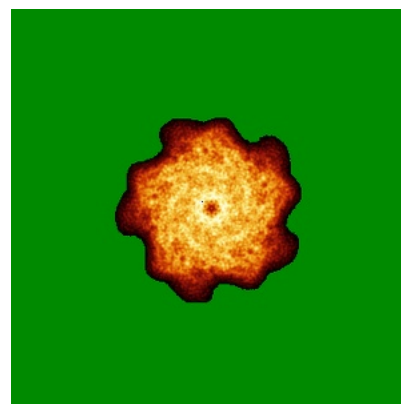
6.4.1 Primary map



X

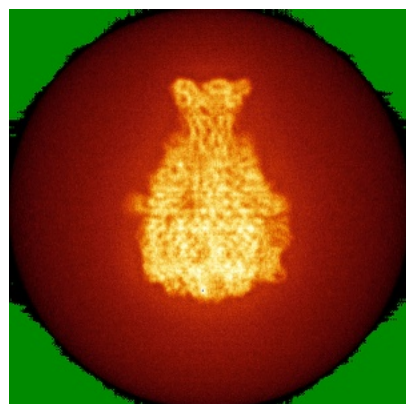


Y

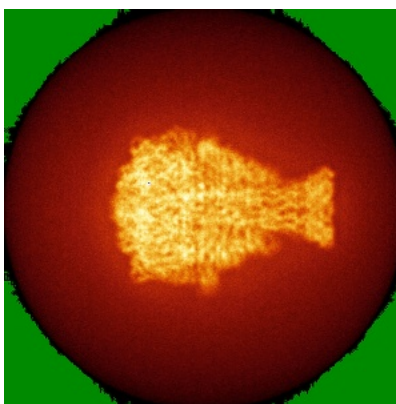


Z

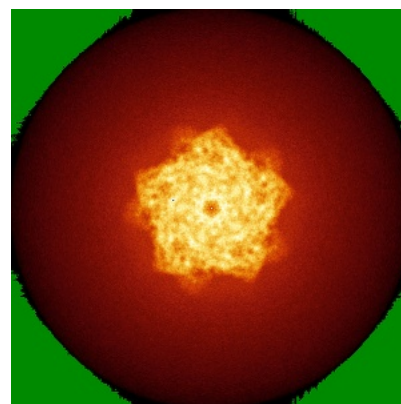
6.4.2 Raw map



X



Y



Z

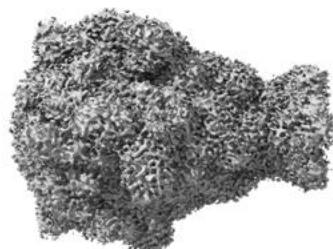
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

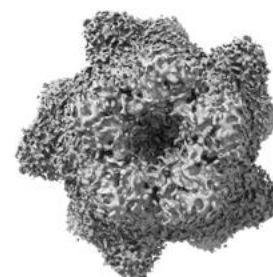
6.5.1 Primary map



X



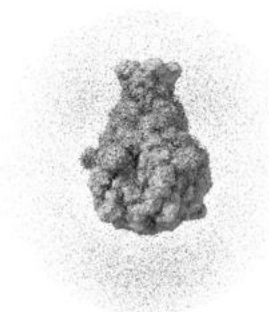
Y



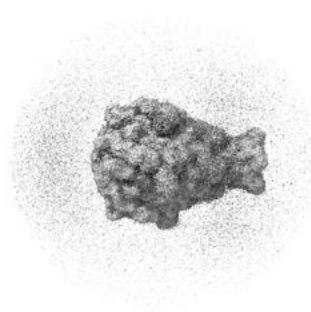
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00379. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

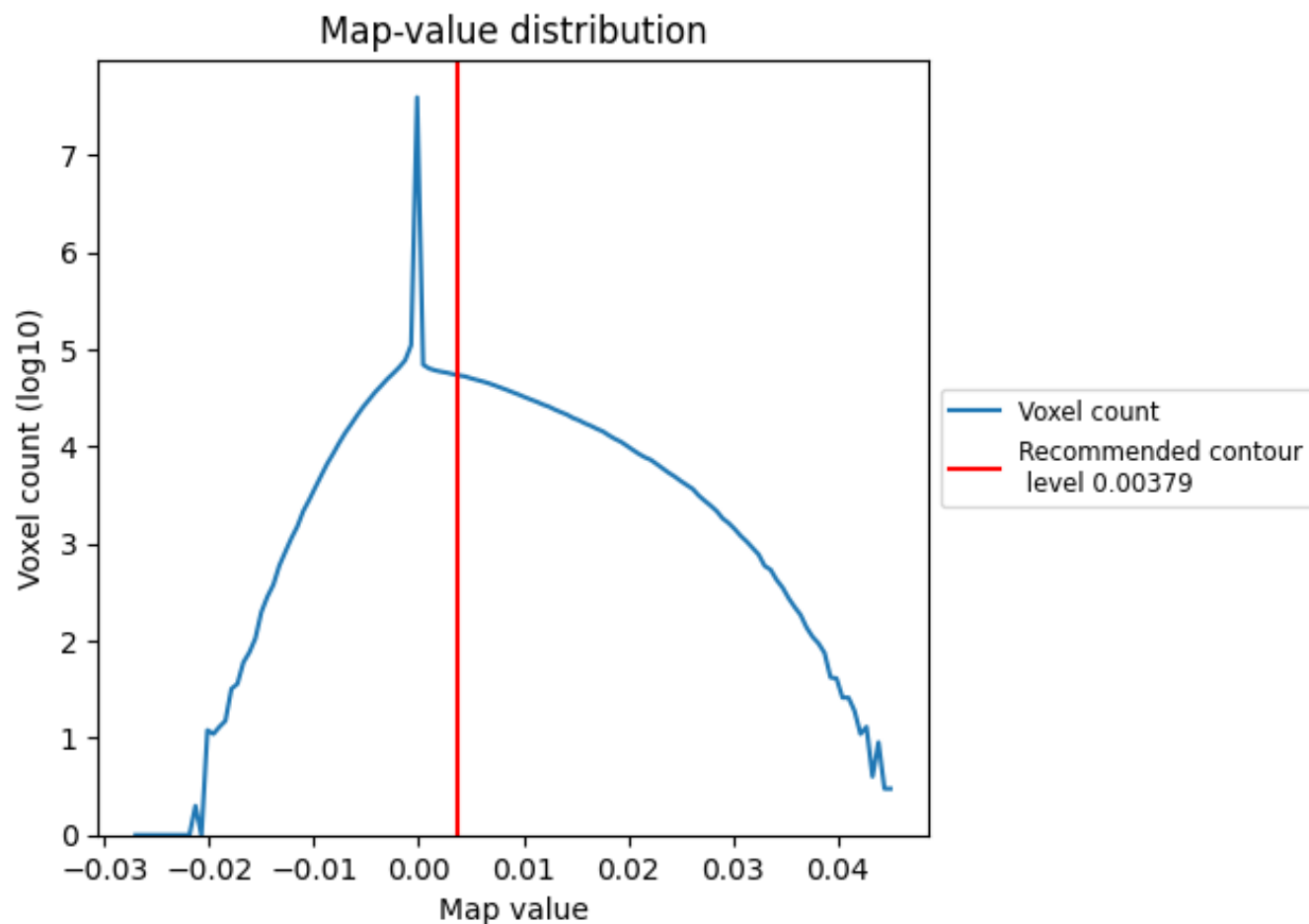
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

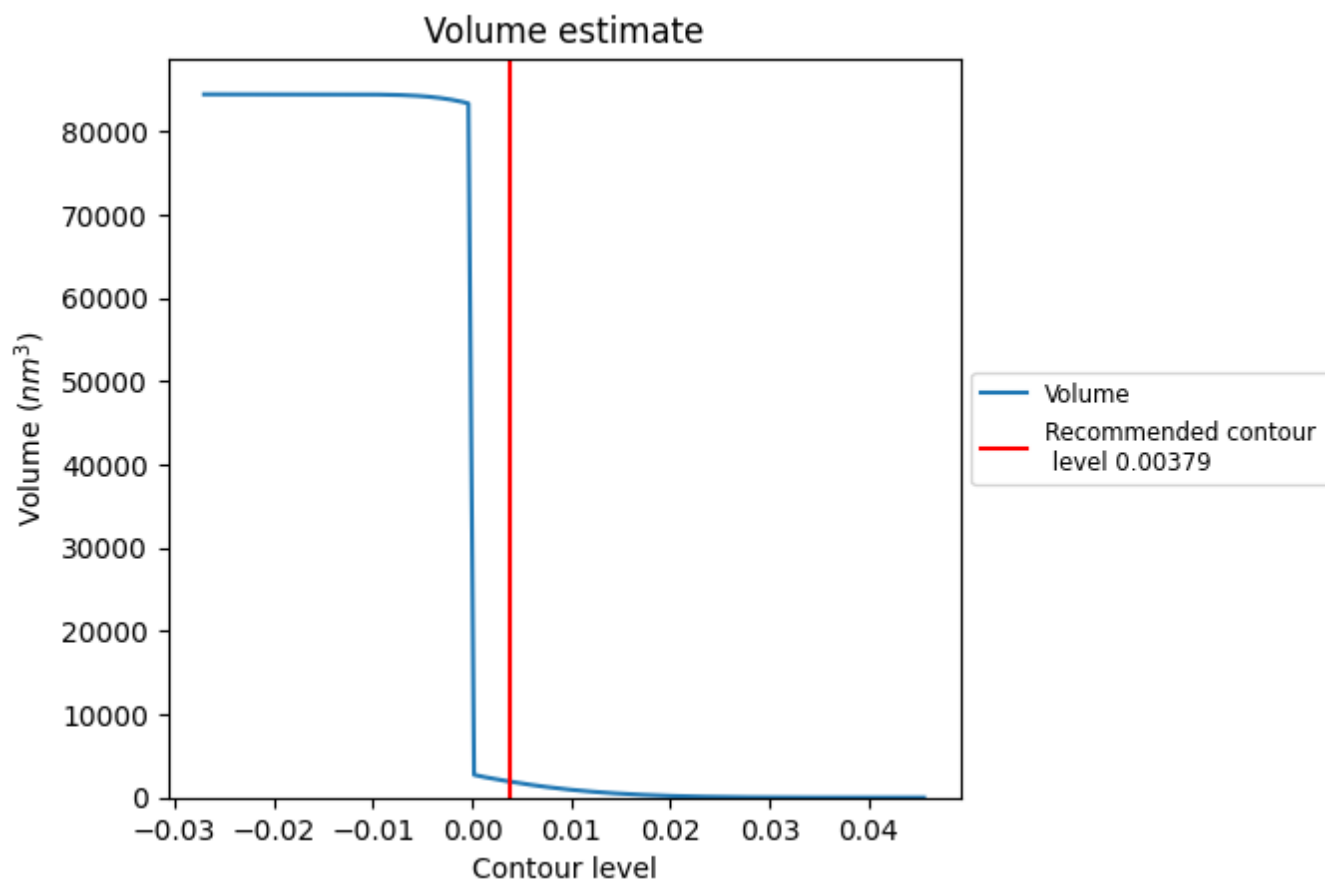
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

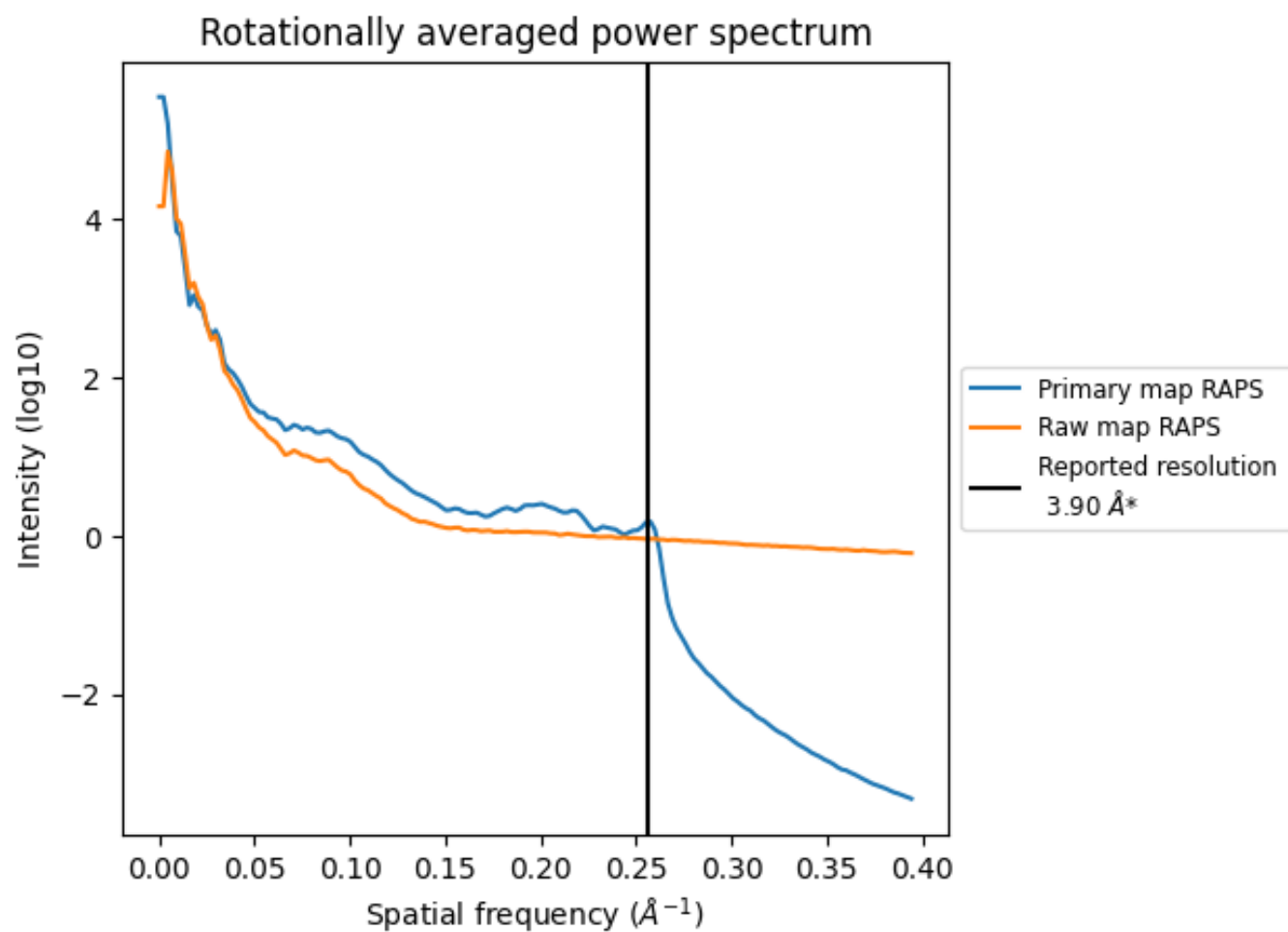
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1929 nm^3 ; this corresponds to an approximate mass of 1743 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

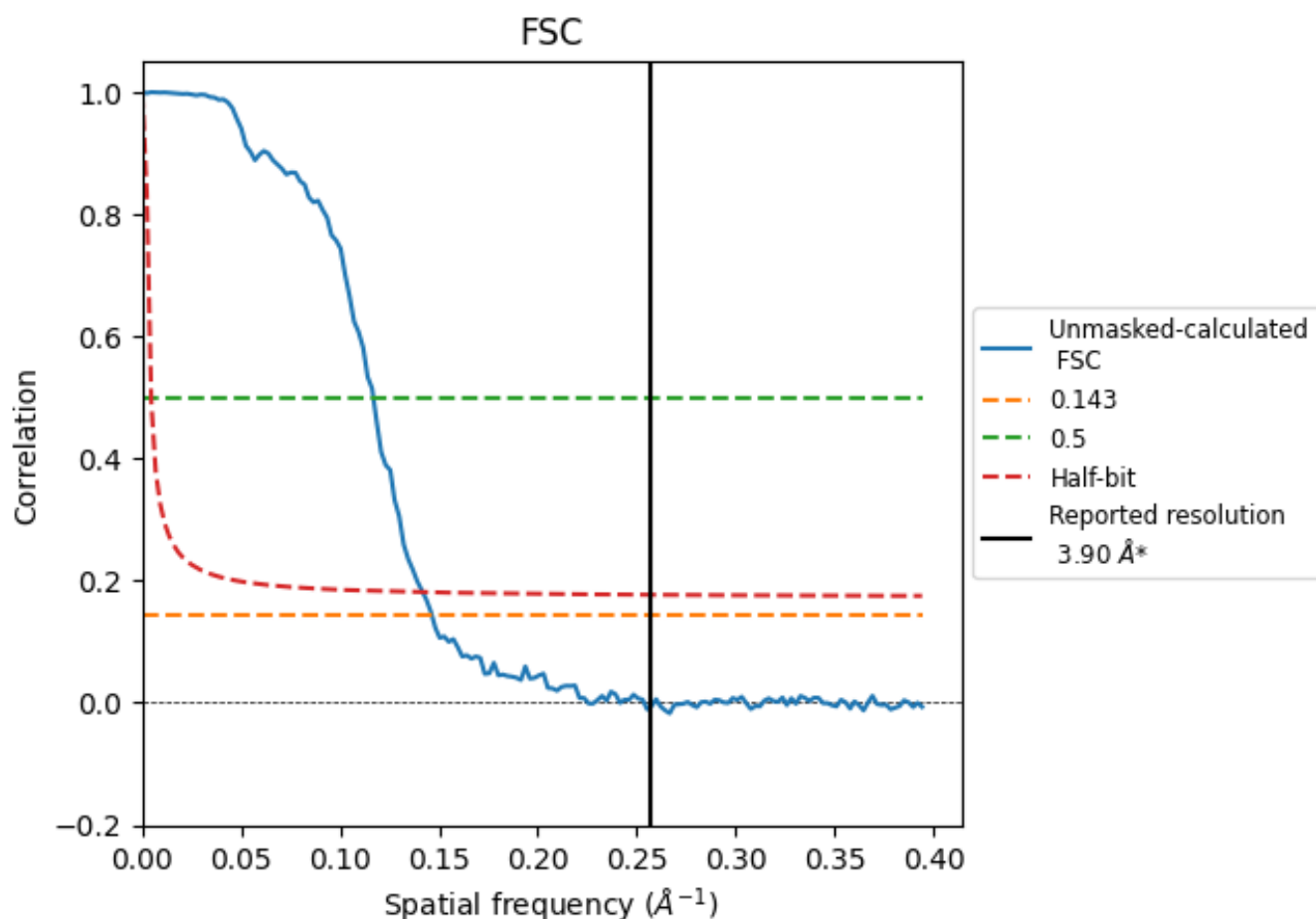


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

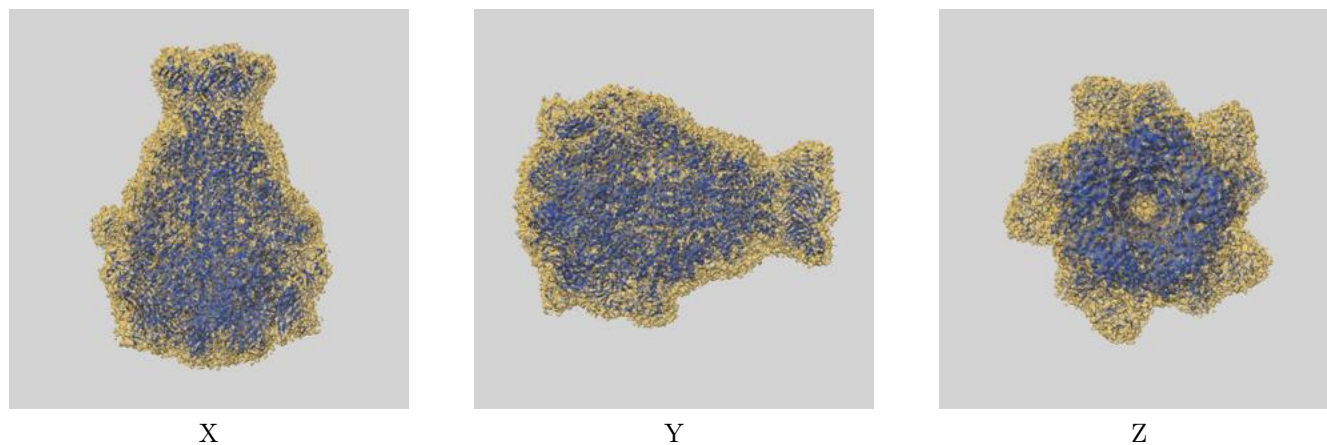
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.83	8.55	7.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.83 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

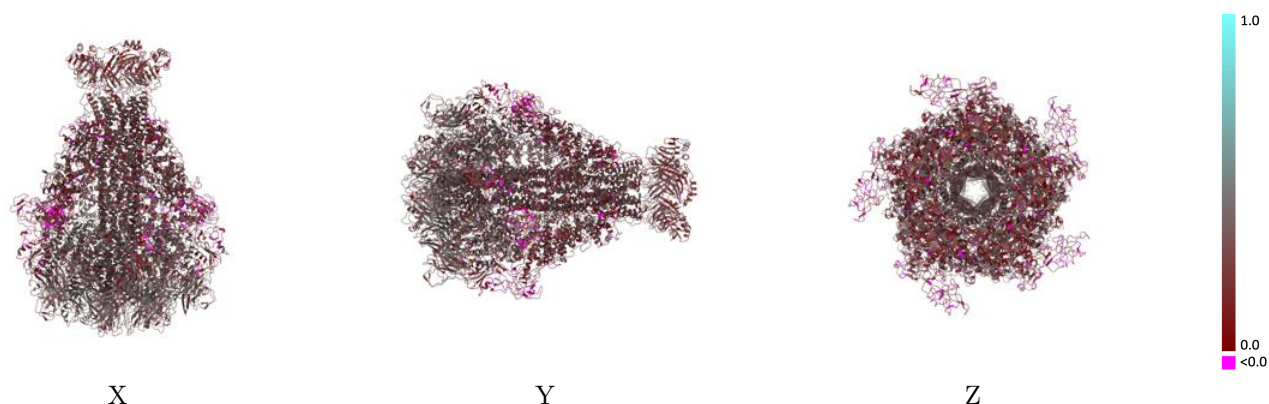
This section contains information regarding the fit between EMDB map EMD-48372 and PDB model 9MLH. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



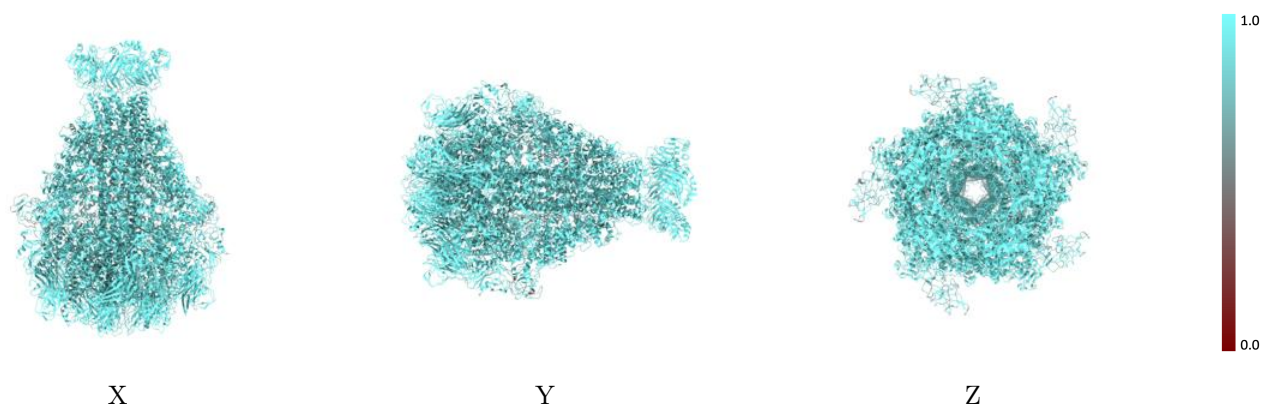
The images above show the 3D surface view of the map at the recommended contour level 0.00379 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



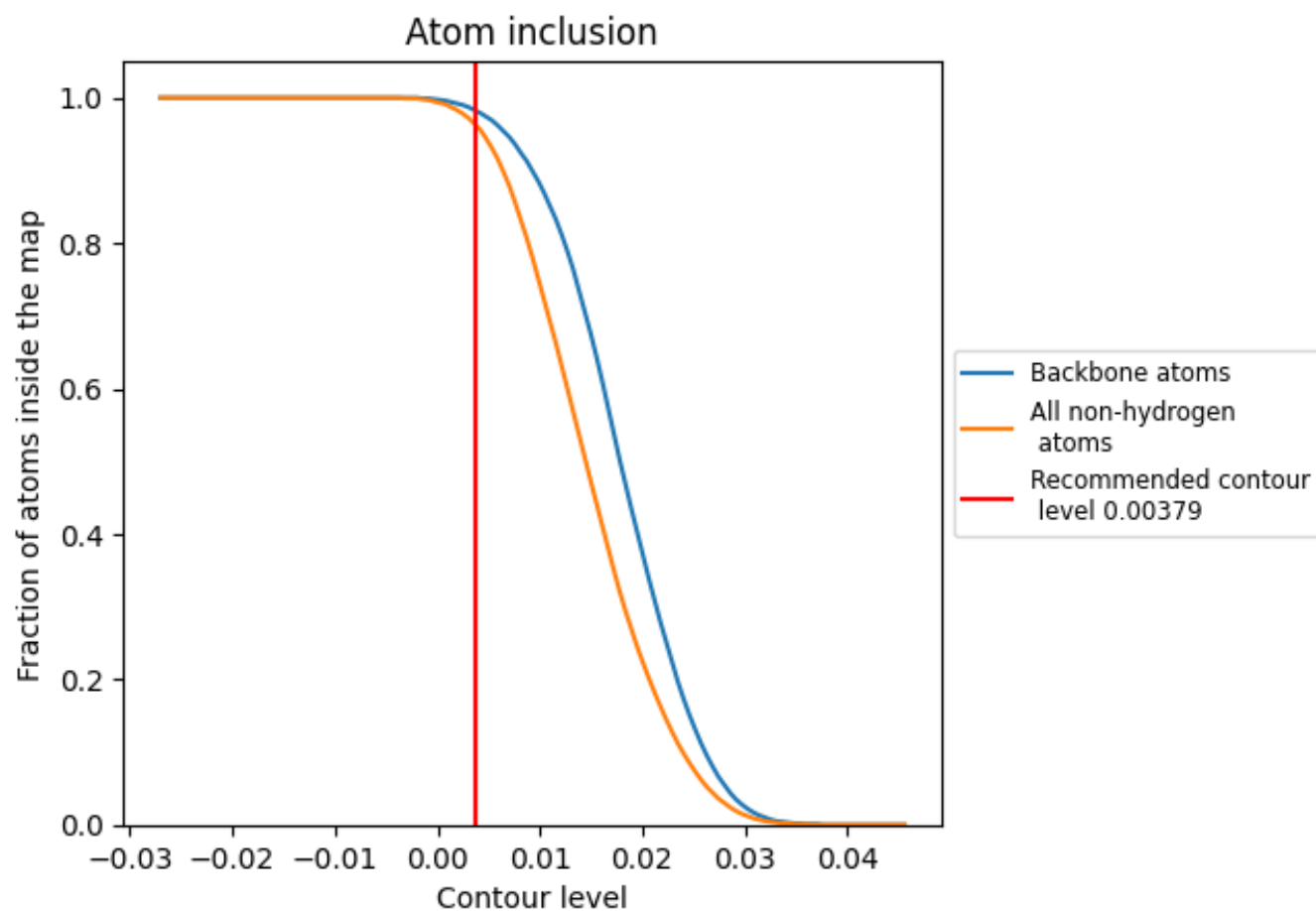
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00379).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00379) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9620	0.3000
A	0.9610	0.2990
B	0.9630	0.2990
C	0.9620	0.3000
D	0.9630	0.3000
E	0.9630	0.3010

