



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:35 PM UTC

PDB ID : 8TQE / pdb_00008tqe
EMDB ID : EMD-41503
Title : XptA2 wild type
Authors : Martin, C.L.; Binshtein, E.M.; Aller, S.G.
Deposited on : 2023-08-07
Resolution : 3.10 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

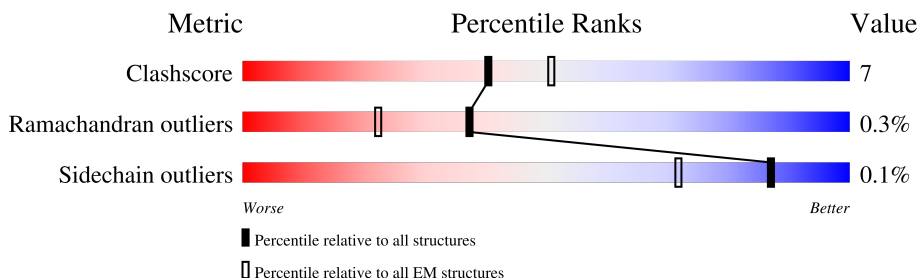
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

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

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100035 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2537	Total 20007	C 12625	N 3415	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 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	HIS	PRO	conflict	UNP N1NRW3
A	343	ASN	HIS	conflict	UNP N1NRW3
A	344	ILE	VAL	conflict	UNP N1NRW3
A	360	ARG	CYS	conflict	UNP N1NRW3
A	365	VAL	ILE	conflict	UNP N1NRW3
A	377	ALA	SER	conflict	UNP N1NRW3
A	379	PRO	THR	conflict	UNP N1NRW3
A	391	ILE	VAL	conflict	UNP N1NRW3
A	407	SER	ASN	conflict	UNP N1NRW3
A	410	LYS	ARG	conflict	UNP N1NRW3
A	566	VAL	ILE	conflict	UNP N1NRW3
A	583	ALA	THR	conflict	UNP N1NRW3
A	586	THR	ILE	conflict	UNP N1NRW3
A	587	ILE	LEU	conflict	UNP N1NRW3
A	592	PHE	PRO	conflict	UNP N1NRW3
A	606	VAL	ALA	conflict	UNP N1NRW3
A	620	LEU	PHE	conflict	UNP N1NRW3
A	637	PRO	SER	conflict	UNP N1NRW3
A	682	ASN	THR	conflict	UNP N1NRW3
A	686	SER	ARG	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	695	HIS	SER	conflict	UNP N1NRW3
A	696	ASN	ASP	conflict	UNP N1NRW3
A	736	ASP	ASN	conflict	UNP N1NRW3
A	742	THR	MET	conflict	UNP N1NRW3
A	748	SER	THR	conflict	UNP N1NRW3
A	750	ASN	SER	conflict	UNP N1NRW3
A	751	ALA	ASP	conflict	UNP N1NRW3
A	752	ASN	GLU	conflict	UNP N1NRW3
A	788	GLY	ASP	conflict	UNP N1NRW3
A	790	ALA	VAL	conflict	UNP N1NRW3
A	795	LYS	ARG	conflict	UNP N1NRW3
A	796	ASN	SER	conflict	UNP N1NRW3
A	911	SER	ALA	conflict	UNP N1NRW3
A	914	GLU	LYS	conflict	UNP N1NRW3
A	923	GLU	ALA	conflict	UNP N1NRW3
A	1067	LYS	GLN	conflict	UNP N1NRW3
A	1075	ASP	GLU	conflict	UNP N1NRW3
A	1126	ASP	ASN	conflict	UNP N1NRW3
A	1250	LYS	VAL	conflict	UNP N1NRW3
A	1253	SER	PRO	conflict	UNP N1NRW3
A	1257	GLY	ASP	conflict	UNP N1NRW3
A	1258	SER	ASN	conflict	UNP N1NRW3
A	1514	ILE	VAL	conflict	UNP N1NRW3
A	1519	MET	VAL	conflict	UNP N1NRW3
A	1877	ASN	TYR	conflict	UNP N1NRW3
A	1880	MET	THR	conflict	UNP N1NRW3
A	1884	ILE	VAL	conflict	UNP N1NRW3
A	1920	THR	ALA	conflict	UNP N1NRW3
A	1943	GLY	VAL	conflict	UNP N1NRW3
A	1947	GLN	HIS	conflict	UNP N1NRW3
A	1959	MET	ALA	conflict	UNP N1NRW3
A	1961	GLY	ASP	conflict	UNP N1NRW3
A	1962	ARG	ASN	conflict	UNP N1NRW3
A	1964	GLY	GLU	conflict	UNP N1NRW3
A	1966	SER	ALA	conflict	UNP N1NRW3
A	1967	LYS	THR	conflict	UNP N1NRW3
A	1968	ASN	GLN	conflict	UNP N1NRW3
A	1969	LEU	PRO	conflict	UNP N1NRW3
A	2057	THR	ALA	conflict	UNP N1NRW3
A	2149	LEU	PHE	conflict	UNP N1NRW3
A	2161	VAL	ALA	conflict	UNP N1NRW3
A	2164	ILE	VAL	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2178	LEU	PHE	conflict	UNP N1NRW3
A	2430	LEU	PHE	conflict	UNP N1NRW3
B	172	HIS	PRO	conflict	UNP N1NRW3
B	343	ASN	HIS	conflict	UNP N1NRW3
B	344	ILE	VAL	conflict	UNP N1NRW3
B	360	ARG	CYS	conflict	UNP N1NRW3
B	365	VAL	ILE	conflict	UNP N1NRW3
B	377	ALA	SER	conflict	UNP N1NRW3
B	379	PRO	THR	conflict	UNP N1NRW3
B	391	ILE	VAL	conflict	UNP N1NRW3
B	407	SER	ASN	conflict	UNP N1NRW3
B	410	LYS	ARG	conflict	UNP N1NRW3
B	566	VAL	ILE	conflict	UNP N1NRW3
B	583	ALA	THR	conflict	UNP N1NRW3
B	586	THR	ILE	conflict	UNP N1NRW3
B	587	ILE	LEU	conflict	UNP N1NRW3
B	592	PHE	PRO	conflict	UNP N1NRW3
B	606	VAL	ALA	conflict	UNP N1NRW3
B	620	LEU	PHE	conflict	UNP N1NRW3
B	637	PRO	SER	conflict	UNP N1NRW3
B	682	ASN	THR	conflict	UNP N1NRW3
B	686	SER	ARG	conflict	UNP N1NRW3
B	695	HIS	SER	conflict	UNP N1NRW3
B	696	ASN	ASP	conflict	UNP N1NRW3
B	736	ASP	ASN	conflict	UNP N1NRW3
B	742	THR	MET	conflict	UNP N1NRW3
B	748	SER	THR	conflict	UNP N1NRW3
B	750	ASN	SER	conflict	UNP N1NRW3
B	751	ALA	ASP	conflict	UNP N1NRW3
B	752	ASN	GLU	conflict	UNP N1NRW3
B	788	GLY	ASP	conflict	UNP N1NRW3
B	790	ALA	VAL	conflict	UNP N1NRW3
B	795	LYS	ARG	conflict	UNP N1NRW3
B	796	ASN	SER	conflict	UNP N1NRW3
B	911	SER	ALA	conflict	UNP N1NRW3
B	914	GLU	LYS	conflict	UNP N1NRW3
B	923	GLU	ALA	conflict	UNP N1NRW3
B	1067	LYS	GLN	conflict	UNP N1NRW3
B	1075	ASP	GLU	conflict	UNP N1NRW3
B	1126	ASP	ASN	conflict	UNP N1NRW3
B	1250	LYS	VAL	conflict	UNP N1NRW3
B	1253	SER	PRO	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1257	GLY	ASP	conflict	UNP N1NRW3
B	1258	SER	ASN	conflict	UNP N1NRW3
B	1514	ILE	VAL	conflict	UNP N1NRW3
B	1519	MET	VAL	conflict	UNP N1NRW3
B	1877	ASN	TYR	conflict	UNP N1NRW3
B	1880	MET	THR	conflict	UNP N1NRW3
B	1884	ILE	VAL	conflict	UNP N1NRW3
B	1920	THR	ALA	conflict	UNP N1NRW3
B	1943	GLY	VAL	conflict	UNP N1NRW3
B	1947	GLN	HIS	conflict	UNP N1NRW3
B	1959	MET	ALA	conflict	UNP N1NRW3
B	1961	GLY	ASP	conflict	UNP N1NRW3
B	1962	ARG	ASN	conflict	UNP N1NRW3
B	1964	GLY	GLU	conflict	UNP N1NRW3
B	1966	SER	ALA	conflict	UNP N1NRW3
B	1967	LYS	THR	conflict	UNP N1NRW3
B	1968	ASN	GLN	conflict	UNP N1NRW3
B	1969	LEU	PRO	conflict	UNP N1NRW3
B	2057	THR	ALA	conflict	UNP N1NRW3
B	2149	LEU	PHE	conflict	UNP N1NRW3
B	2161	VAL	ALA	conflict	UNP N1NRW3
B	2164	ILE	VAL	conflict	UNP N1NRW3
B	2178	LEU	PHE	conflict	UNP N1NRW3
B	2430	LEU	PHE	conflict	UNP N1NRW3
C	172	HIS	PRO	conflict	UNP N1NRW3
C	343	ASN	HIS	conflict	UNP N1NRW3
C	344	ILE	VAL	conflict	UNP N1NRW3
C	360	ARG	CYS	conflict	UNP N1NRW3
C	365	VAL	ILE	conflict	UNP N1NRW3
C	377	ALA	SER	conflict	UNP N1NRW3
C	379	PRO	THR	conflict	UNP N1NRW3
C	391	ILE	VAL	conflict	UNP N1NRW3
C	407	SER	ASN	conflict	UNP N1NRW3
C	410	LYS	ARG	conflict	UNP N1NRW3
C	566	VAL	ILE	conflict	UNP N1NRW3
C	583	ALA	THR	conflict	UNP N1NRW3
C	586	THR	ILE	conflict	UNP N1NRW3
C	587	ILE	LEU	conflict	UNP N1NRW3
C	592	PHE	PRO	conflict	UNP N1NRW3
C	606	VAL	ALA	conflict	UNP N1NRW3
C	620	LEU	PHE	conflict	UNP N1NRW3
C	637	PRO	SER	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	682	ASN	THR	conflict	UNP N1NRW3
C	686	SER	ARG	conflict	UNP N1NRW3
C	695	HIS	SER	conflict	UNP N1NRW3
C	696	ASN	ASP	conflict	UNP N1NRW3
C	736	ASP	ASN	conflict	UNP N1NRW3
C	742	THR	MET	conflict	UNP N1NRW3
C	748	SER	THR	conflict	UNP N1NRW3
C	750	ASN	SER	conflict	UNP N1NRW3
C	751	ALA	ASP	conflict	UNP N1NRW3
C	752	ASN	GLU	conflict	UNP N1NRW3
C	788	GLY	ASP	conflict	UNP N1NRW3
C	790	ALA	VAL	conflict	UNP N1NRW3
C	795	LYS	ARG	conflict	UNP N1NRW3
C	796	ASN	SER	conflict	UNP N1NRW3
C	911	SER	ALA	conflict	UNP N1NRW3
C	914	GLU	LYS	conflict	UNP N1NRW3
C	923	GLU	ALA	conflict	UNP N1NRW3
C	1067	LYS	GLN	conflict	UNP N1NRW3
C	1075	ASP	GLU	conflict	UNP N1NRW3
C	1126	ASP	ASN	conflict	UNP N1NRW3
C	1250	LYS	VAL	conflict	UNP N1NRW3
C	1253	SER	PRO	conflict	UNP N1NRW3
C	1257	GLY	ASP	conflict	UNP N1NRW3
C	1258	SER	ASN	conflict	UNP N1NRW3
C	1514	ILE	VAL	conflict	UNP N1NRW3
C	1519	MET	VAL	conflict	UNP N1NRW3
C	1877	ASN	TYR	conflict	UNP N1NRW3
C	1880	MET	THR	conflict	UNP N1NRW3
C	1884	ILE	VAL	conflict	UNP N1NRW3
C	1920	THR	ALA	conflict	UNP N1NRW3
C	1943	GLY	VAL	conflict	UNP N1NRW3
C	1947	GLN	HIS	conflict	UNP N1NRW3
C	1959	MET	ALA	conflict	UNP N1NRW3
C	1961	GLY	ASP	conflict	UNP N1NRW3
C	1962	ARG	ASN	conflict	UNP N1NRW3
C	1964	GLY	GLU	conflict	UNP N1NRW3
C	1966	SER	ALA	conflict	UNP N1NRW3
C	1967	LYS	THR	conflict	UNP N1NRW3
C	1968	ASN	GLN	conflict	UNP N1NRW3
C	1969	LEU	PRO	conflict	UNP N1NRW3
C	2057	THR	ALA	conflict	UNP N1NRW3
C	2149	LEU	PHE	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2161	VAL	ALA	conflict	UNP N1NRW3
C	2164	ILE	VAL	conflict	UNP N1NRW3
C	2178	LEU	PHE	conflict	UNP N1NRW3
C	2430	LEU	PHE	conflict	UNP N1NRW3
D	172	HIS	PRO	conflict	UNP N1NRW3
D	343	ASN	HIS	conflict	UNP N1NRW3
D	344	ILE	VAL	conflict	UNP N1NRW3
D	360	ARG	CYS	conflict	UNP N1NRW3
D	365	VAL	ILE	conflict	UNP N1NRW3
D	377	ALA	SER	conflict	UNP N1NRW3
D	379	PRO	THR	conflict	UNP N1NRW3
D	391	ILE	VAL	conflict	UNP N1NRW3
D	407	SER	ASN	conflict	UNP N1NRW3
D	410	LYS	ARG	conflict	UNP N1NRW3
D	566	VAL	ILE	conflict	UNP N1NRW3
D	583	ALA	THR	conflict	UNP N1NRW3
D	586	THR	ILE	conflict	UNP N1NRW3
D	587	ILE	LEU	conflict	UNP N1NRW3
D	592	PHE	PRO	conflict	UNP N1NRW3
D	606	VAL	ALA	conflict	UNP N1NRW3
D	620	LEU	PHE	conflict	UNP N1NRW3
D	637	PRO	SER	conflict	UNP N1NRW3
D	682	ASN	THR	conflict	UNP N1NRW3
D	686	SER	ARG	conflict	UNP N1NRW3
D	695	HIS	SER	conflict	UNP N1NRW3
D	696	ASN	ASP	conflict	UNP N1NRW3
D	736	ASP	ASN	conflict	UNP N1NRW3
D	742	THR	MET	conflict	UNP N1NRW3
D	748	SER	THR	conflict	UNP N1NRW3
D	750	ASN	SER	conflict	UNP N1NRW3
D	751	ALA	ASP	conflict	UNP N1NRW3
D	752	ASN	GLU	conflict	UNP N1NRW3
D	788	GLY	ASP	conflict	UNP N1NRW3
D	790	ALA	VAL	conflict	UNP N1NRW3
D	795	LYS	ARG	conflict	UNP N1NRW3
D	796	ASN	SER	conflict	UNP N1NRW3
D	911	SER	ALA	conflict	UNP N1NRW3
D	914	GLU	LYS	conflict	UNP N1NRW3
D	923	GLU	ALA	conflict	UNP N1NRW3
D	1067	LYS	GLN	conflict	UNP N1NRW3
D	1075	ASP	GLU	conflict	UNP N1NRW3
D	1126	ASP	ASN	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1250	LYS	VAL	conflict	UNP N1NRW3
D	1253	SER	PRO	conflict	UNP N1NRW3
D	1257	GLY	ASP	conflict	UNP N1NRW3
D	1258	SER	ASN	conflict	UNP N1NRW3
D	1514	ILE	VAL	conflict	UNP N1NRW3
D	1519	MET	VAL	conflict	UNP N1NRW3
D	1877	ASN	TYR	conflict	UNP N1NRW3
D	1880	MET	THR	conflict	UNP N1NRW3
D	1884	ILE	VAL	conflict	UNP N1NRW3
D	1920	THR	ALA	conflict	UNP N1NRW3
D	1943	GLY	VAL	conflict	UNP N1NRW3
D	1947	GLN	HIS	conflict	UNP N1NRW3
D	1959	MET	ALA	conflict	UNP N1NRW3
D	1961	GLY	ASP	conflict	UNP N1NRW3
D	1962	ARG	ASN	conflict	UNP N1NRW3
D	1964	GLY	GLU	conflict	UNP N1NRW3
D	1966	SER	ALA	conflict	UNP N1NRW3
D	1967	LYS	THR	conflict	UNP N1NRW3
D	1968	ASN	GLN	conflict	UNP N1NRW3
D	1969	LEU	PRO	conflict	UNP N1NRW3
D	2057	THR	ALA	conflict	UNP N1NRW3
D	2149	LEU	PHE	conflict	UNP N1NRW3
D	2161	VAL	ALA	conflict	UNP N1NRW3
D	2164	ILE	VAL	conflict	UNP N1NRW3
D	2178	LEU	PHE	conflict	UNP N1NRW3
D	2430	LEU	PHE	conflict	UNP N1NRW3
E	172	HIS	PRO	conflict	UNP N1NRW3
E	343	ASN	HIS	conflict	UNP N1NRW3
E	344	ILE	VAL	conflict	UNP N1NRW3
E	360	ARG	CYS	conflict	UNP N1NRW3
E	365	VAL	ILE	conflict	UNP N1NRW3
E	377	ALA	SER	conflict	UNP N1NRW3
E	379	PRO	THR	conflict	UNP N1NRW3
E	391	ILE	VAL	conflict	UNP N1NRW3
E	407	SER	ASN	conflict	UNP N1NRW3
E	410	LYS	ARG	conflict	UNP N1NRW3
E	566	VAL	ILE	conflict	UNP N1NRW3
E	583	ALA	THR	conflict	UNP N1NRW3
E	586	THR	ILE	conflict	UNP N1NRW3
E	587	ILE	LEU	conflict	UNP N1NRW3
E	592	PHE	PRO	conflict	UNP N1NRW3
E	606	VAL	ALA	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	620	LEU	PHE	conflict	UNP N1NRW3
E	637	PRO	SER	conflict	UNP N1NRW3
E	682	ASN	THR	conflict	UNP N1NRW3
E	686	SER	ARG	conflict	UNP N1NRW3
E	695	HIS	SER	conflict	UNP N1NRW3
E	696	ASN	ASP	conflict	UNP N1NRW3
E	736	ASP	ASN	conflict	UNP N1NRW3
E	742	THR	MET	conflict	UNP N1NRW3
E	748	SER	THR	conflict	UNP N1NRW3
E	750	ASN	SER	conflict	UNP N1NRW3
E	751	ALA	ASP	conflict	UNP N1NRW3
E	752	ASN	GLU	conflict	UNP N1NRW3
E	788	GLY	ASP	conflict	UNP N1NRW3
E	790	ALA	VAL	conflict	UNP N1NRW3
E	795	LYS	ARG	conflict	UNP N1NRW3
E	796	ASN	SER	conflict	UNP N1NRW3
E	911	SER	ALA	conflict	UNP N1NRW3
E	914	GLU	LYS	conflict	UNP N1NRW3
E	923	GLU	ALA	conflict	UNP N1NRW3
E	1067	LYS	GLN	conflict	UNP N1NRW3
E	1075	ASP	GLU	conflict	UNP N1NRW3
E	1126	ASP	ASN	conflict	UNP N1NRW3
E	1250	LYS	VAL	conflict	UNP N1NRW3
E	1253	SER	PRO	conflict	UNP N1NRW3
E	1257	GLY	ASP	conflict	UNP N1NRW3
E	1258	SER	ASN	conflict	UNP N1NRW3
E	1514	ILE	VAL	conflict	UNP N1NRW3
E	1519	MET	VAL	conflict	UNP N1NRW3
E	1877	ASN	TYR	conflict	UNP N1NRW3
E	1880	MET	THR	conflict	UNP N1NRW3
E	1884	ILE	VAL	conflict	UNP N1NRW3
E	1920	THR	ALA	conflict	UNP N1NRW3
E	1943	GLY	VAL	conflict	UNP N1NRW3
E	1947	GLN	HIS	conflict	UNP N1NRW3
E	1959	MET	ALA	conflict	UNP N1NRW3
E	1961	GLY	ASP	conflict	UNP N1NRW3
E	1962	ARG	ASN	conflict	UNP N1NRW3
E	1964	GLY	GLU	conflict	UNP N1NRW3
E	1966	SER	ALA	conflict	UNP N1NRW3
E	1967	LYS	THR	conflict	UNP N1NRW3
E	1968	ASN	GLN	conflict	UNP N1NRW3
E	1969	LEU	PRO	conflict	UNP N1NRW3

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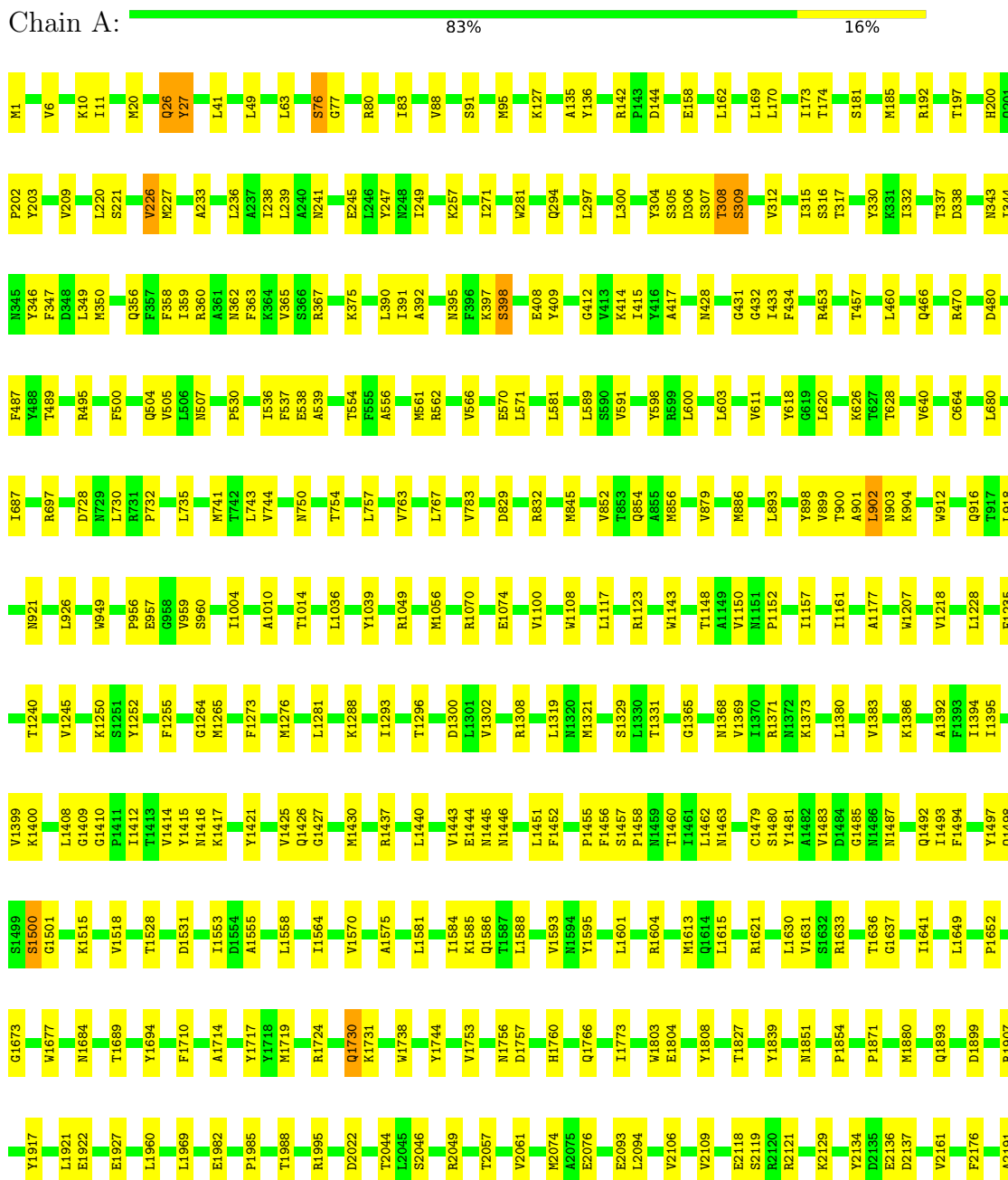
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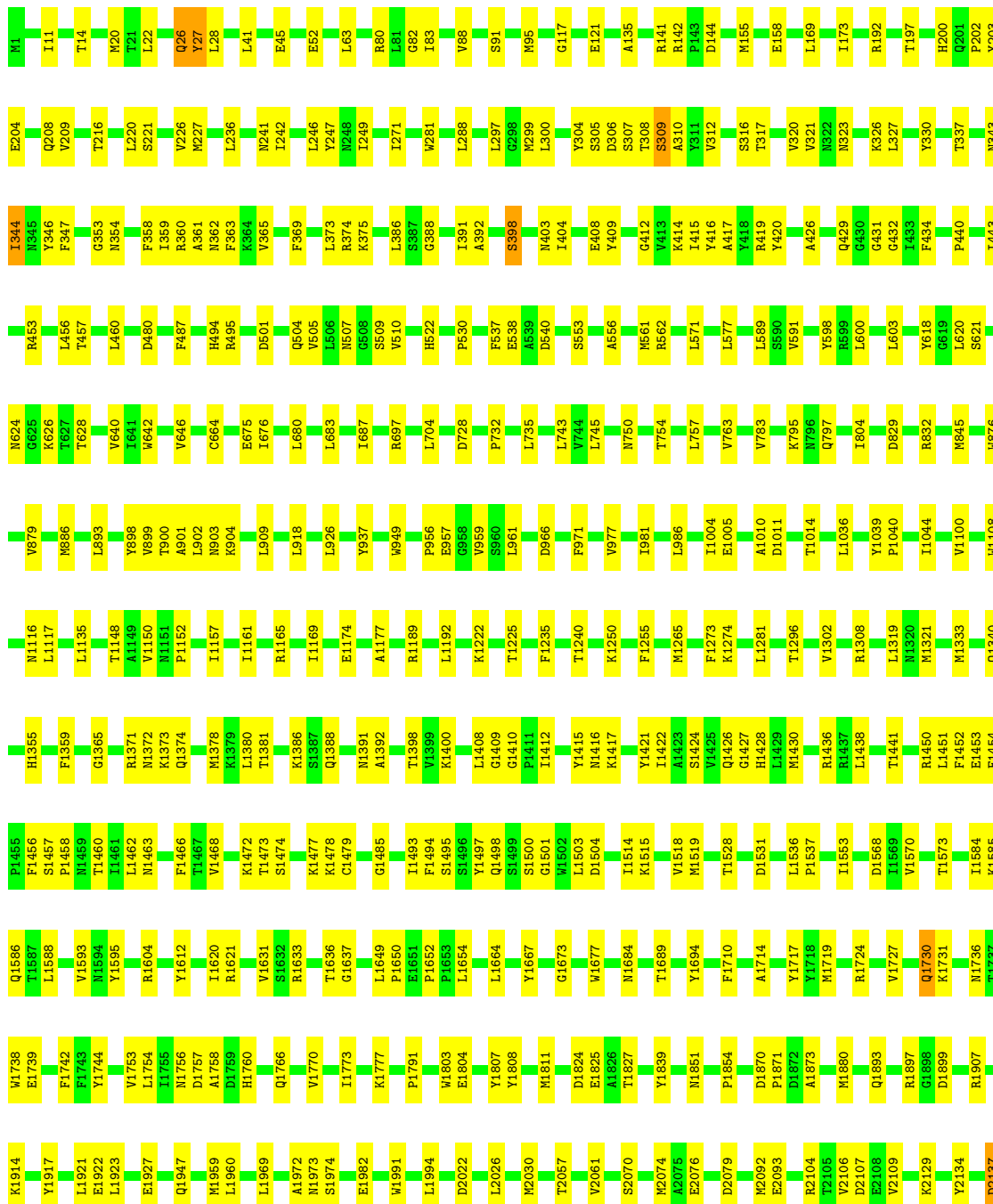
Chain	Residue	Modelled	Actual	Comment	Reference
E	2057	THR	ALA	conflict	UNP N1NRW3
E	2149	LEU	PHE	conflict	UNP N1NRW3
E	2161	VAL	ALA	conflict	UNP N1NRW3
E	2164	ILE	VAL	conflict	UNP N1NRW3
E	2178	LEU	PHE	conflict	UNP N1NRW3
E	2430	LEU	PHE	conflict	UNP N1NRW3

3 Residue-property plots

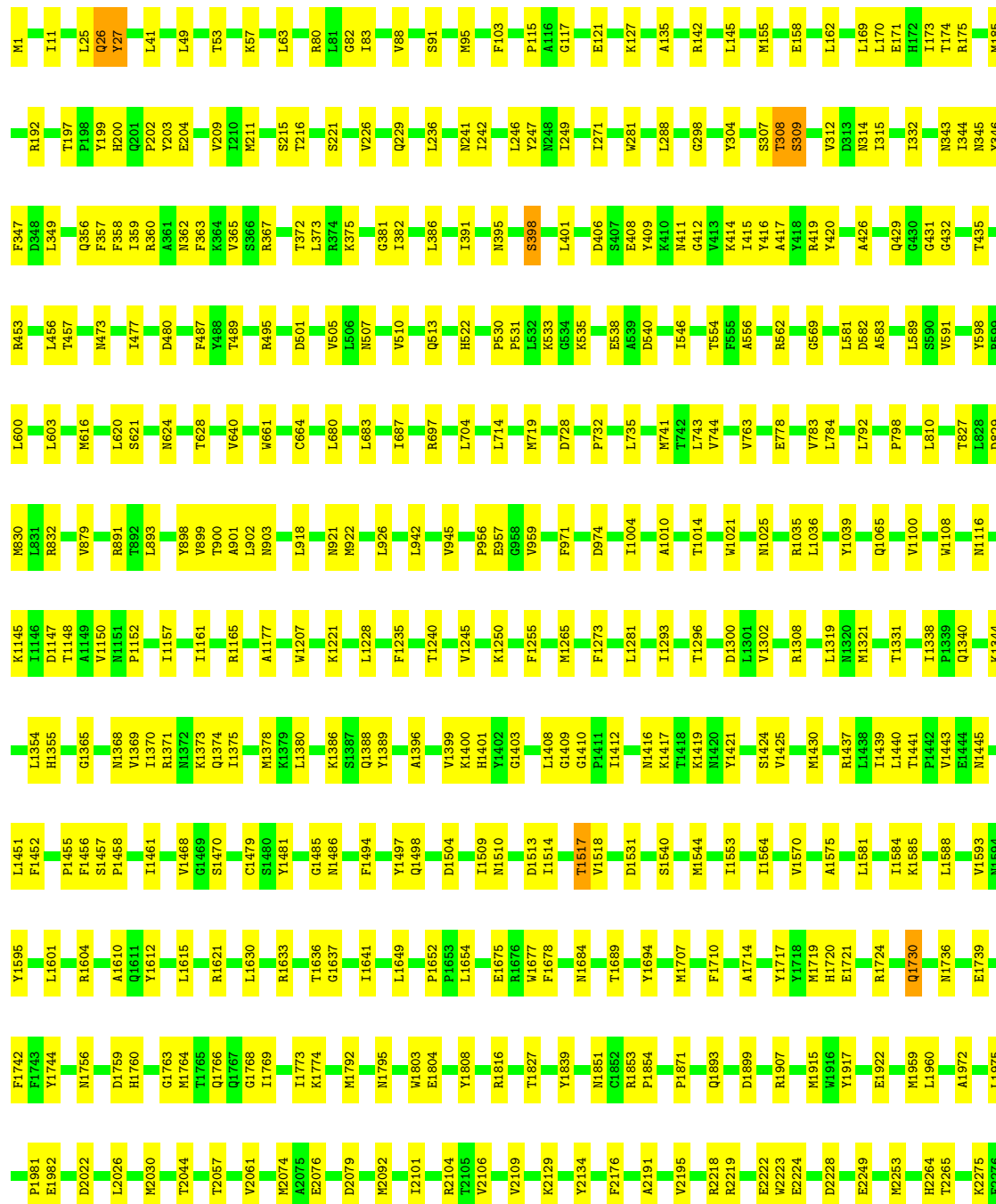
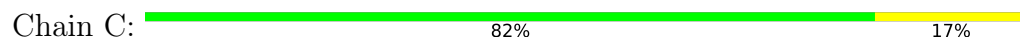
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

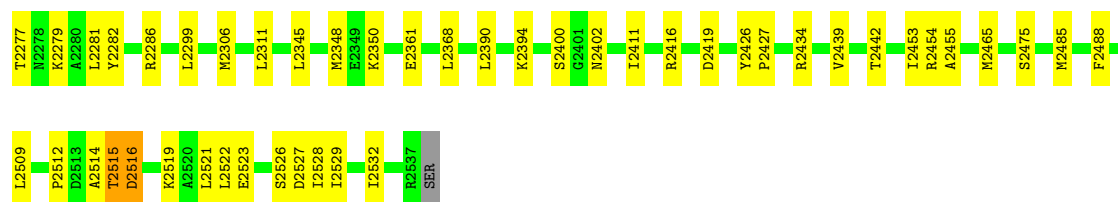
• Molecule 1: XptA2



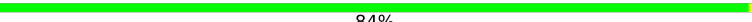
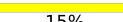


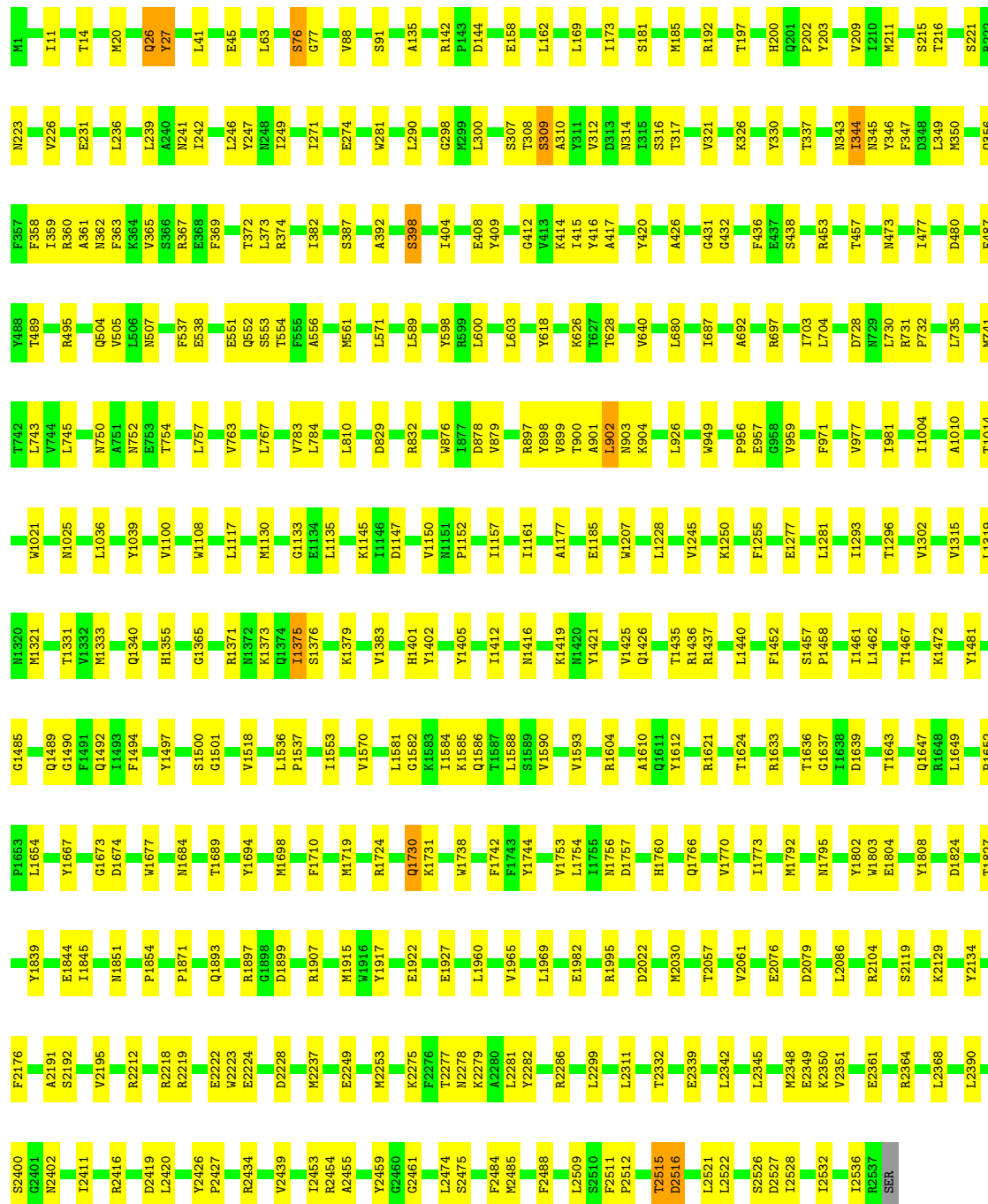
- Molecule 1: XptA2





• Molecule 1: XptA2

Chain D:  84%  15%



Chain E: 83% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	198591	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

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	0.19	0/20413	0.41	10/27714 (0.0%)
1	B	0.19	0/20413	0.40	7/27714 (0.0%)
1	C	0.19	0/20413	0.41	8/27714 (0.0%)
1	D	0.19	0/20413	0.41	8/27714 (0.0%)
1	E	0.18	0/20413	0.40	6/27714 (0.0%)
All	All	0.19	0/102065	0.41	39/138570 (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	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2515	THR	CA-C-N	15.35	149.34	121.70
1	D	2515	THR	C-N-CA	15.35	149.34	121.70
1	D	26	GLN	CA-C-N	14.95	148.61	121.70
1	D	26	GLN	C-N-CA	14.95	148.61	121.70
1	B	26	GLN	CA-C-N	14.73	148.22	121.70
1	B	26	GLN	C-N-CA	14.73	148.22	121.70
1	E	26	GLN	CA-C-N	14.71	148.18	121.70
1	E	26	GLN	C-N-CA	14.71	148.18	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLN	CA-C-N	14.63	148.03	121.70
1	C	26	GLN	C-N-CA	14.63	148.03	121.70
1	A	26	GLN	CA-C-N	14.61	148.00	121.70
1	A	26	GLN	C-N-CA	14.61	148.00	121.70
1	B	2515	THR	CA-C-N	14.42	147.65	121.70
1	B	2515	THR	C-N-CA	14.42	147.65	121.70
1	C	2515	THR	CA-C-N	14.26	147.36	121.70
1	C	2515	THR	C-N-CA	14.26	147.36	121.70
1	A	2515	THR	CA-C-N	14.14	147.15	121.70
1	A	2515	THR	C-N-CA	14.14	147.15	121.70
1	E	2515	THR	CA-C-N	14.07	147.03	121.70
1	E	2515	THR	C-N-CA	14.07	147.03	121.70
1	D	312	VAL	CA-C-N	10.13	139.93	121.70
1	D	312	VAL	C-N-CA	10.13	139.93	121.70
1	B	312	VAL	CA-C-N	9.79	139.32	121.70
1	B	312	VAL	C-N-CA	9.79	139.32	121.70
1	A	312	VAL	CA-C-N	9.76	139.26	121.70
1	A	312	VAL	C-N-CA	9.76	139.26	121.70
1	C	312	VAL	CA-C-N	9.74	139.24	121.70
1	C	312	VAL	C-N-CA	9.74	139.24	121.70
1	E	312	VAL	CA-C-N	9.52	138.83	121.70
1	E	312	VAL	C-N-CA	9.52	138.83	121.70
1	C	798	PRO	N-CD-CG	-7.93	91.30	103.20
1	B	2137	ASP	CB-CA-C	-6.24	109.39	116.63
1	D	76	SER	CA-C-N	5.71	131.97	121.70
1	D	76	SER	C-N-CA	5.71	131.97	121.70
1	A	76	SER	CA-C-N	5.49	131.58	121.70
1	A	76	SER	C-N-CA	5.49	131.58	121.70
1	A	1500	SER	CB-CA-C	-5.09	110.31	117.23
1	A	1386	LYS	CB-CA-C	-5.06	109.77	115.79
1	C	1386	LYS	CB-CA-C	-5.00	109.84	115.79

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	B	1457	SER	Peptide
1	B	398	SER	Peptide
1	C	398	SER	Peptide
1	D	398	SER	Peptide
1	E	1457	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	398	SER	Peptide

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	20007	0	19592	287	0
1	B	20007	0	19592	314	0
1	C	20007	0	19592	299	0
1	D	20007	0	19592	266	0
1	E	20007	0	19592	290	0
All	All	100035	0	97960	1376	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 7.

All (1376) 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:D:2515:THR:H	1:D:2516:ASP:HB2	1.36	0.90
1:A:2515:THR:H	1:A:2516:ASP:HB2	1.37	0.90
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.36	0.89
1:E:2515:THR:H	1:E:2516:ASP:HB2	1.39	0.88
1:C:2515:THR:H	1:C:2516:ASP:HB2	1.40	0.87
1:B:1391:ASN:HD22	1:B:1416:ASN:HD21	1.21	0.85
1:E:1684:ASN:HB3	1:E:1719:MET:HB2	1.58	0.83
1:A:1440:LEU:HB2	1:A:1452:PHE:HB2	1.60	0.83
1:E:415:ILE:HG21	1:E:432:GLY:H	1.44	0.81
1:B:1684:ASN:HB3	1:B:1719:MET:HB2	1.60	0.81
1:A:338:ASP:OD2	1:A:428:ASN:ND2	2.15	0.80
1:E:1440:LEU:HB2	1:E:1452:PHE:HB2	1.64	0.80
1:D:1383:VAL:HG11	1:D:1467:THR:HB	1.64	0.80
1:C:415:ILE:HG12	1:C:431:GLY:HA3	1.64	0.79
1:E:1485:GLY:HA2	1:E:1494:PHE:HD2	1.47	0.79
1:C:1621:ARG:NH2	1:C:1652:PRO:O	2.16	0.78
1:B:1416:ASN:HB3	1:B:1421:TYR:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.66	0.77
1:C:513:GLN:HE22	1:C:538:GLU:HG2	1.49	0.77
1:D:1150:VAL:HG12	1:D:1152:PRO:HD3	1.66	0.77
1:E:1150:VAL:HG12	1:E:1152:PRO:HD3	1.67	0.77
1:A:1621:ARG:NH2	1:A:1652:PRO:O	2.18	0.77
1:C:1380:LEU:O	1:C:1388:GLN:NE2	2.19	0.76
1:B:1621:ARG:NH2	1:B:1652:PRO:O	2.18	0.76
1:B:135:ALA:HB2	1:B:957:GLU:HB2	1.68	0.76
1:D:1621:ARG:NH2	1:D:1652:PRO:O	2.19	0.75
1:E:1621:ARG:NH2	1:E:1652:PRO:O	2.20	0.75
1:B:415:ILE:HG12	1:B:431:GLY:HA3	1.69	0.75
1:A:1150:VAL:HG12	1:A:1152:PRO:HD3	1.69	0.74
1:E:1946:SER:HB3	1:E:1949:VAL:HG12	1.69	0.74
1:A:365:VAL:HG22	1:A:392:ALA:H	1.53	0.73
1:A:83:ILE:HG12	1:A:1880:MET:HE1	1.71	0.73
1:C:1150:VAL:HG12	1:C:1152:PRO:HD3	1.71	0.73
1:C:1684:ASN:HB3	1:C:1719:MET:HB2	1.69	0.73
1:D:274:GLU:HG2	1:D:1490:GLY:HA2	1.69	0.73
1:C:1612:TYR:HB3	1:C:1654:LEU:HD22	1.71	0.73
1:E:415:ILE:HG21	1:E:432:GLY:N	2.03	0.73
1:E:1485:GLY:HA3	1:E:1493:ILE:HA	1.70	0.72
1:A:1689:THR:O	1:A:1724:ARG:NH2	2.23	0.72
1:B:1689:THR:O	1:B:1724:ARG:NH2	2.22	0.72
1:D:135:ALA:HB2	1:D:957:GLU:HB2	1.72	0.72
1:E:135:ALA:HB2	1:E:957:GLU:HB2	1.71	0.72
1:A:135:ALA:HB2	1:A:957:GLU:HB2	1.72	0.71
1:B:226:VAL:HG21	1:B:879:VAL:HG11	1.72	0.71
1:C:415:ILE:HG21	1:C:432:GLY:H	1.55	0.71
1:C:135:ALA:HB2	1:C:957:GLU:HB2	1.72	0.71
1:E:1689:THR:O	1:E:1724:ARG:NH2	2.23	0.71
1:C:2311:LEU:HD22	1:C:2348:MET:HG2	1.73	0.71
1:E:374:ARG:NH2	1:E:403:ASN:OD1	2.23	0.71
1:E:1500:SER:OG	1:E:1501:GLY:N	2.22	0.71
1:A:2119:SER:HB3	1:A:2237:MET:HE2	1.72	0.70
1:C:2402:ASN:ND2	1:C:2419:ASP:OD2	2.24	0.70
1:E:1373:LYS:HG3	1:E:1412:ILE:HG13	1.72	0.70
1:D:415:ILE:HG12	1:D:431:GLY:HA3	1.73	0.70
1:B:1612:TYR:HB3	1:B:1654:LEU:HD22	1.74	0.70
1:D:1440:LEU:HB2	1:D:1452:PHE:HB2	1.73	0.69
1:E:1808:TYR:HH	1:E:1882:TYR:HH	1.37	0.69
1:A:226:VAL:HG21	1:A:879:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1255:PHE:HB3	1:C:1281:LEU:HG	1.75	0.69
1:D:211:MET:HE3	1:D:211:MET:HA	1.75	0.69
1:A:1383:VAL:H	1:A:1421:TYR:HE1	1.41	0.69
1:C:554:THR:HG22	1:C:556:ALA:H	1.58	0.69
1:D:554:THR:HG22	1:D:556:ALA:H	1.57	0.69
1:C:1678:PHE:HZ	1:C:1707:MET:HE1	1.58	0.69
1:B:404:ILE:HD13	1:B:414:LYS:HD2	1.76	0.68
1:E:1457:SER:HB3	1:E:1458:PRO:HD2	1.75	0.68
1:A:1039:TYR:OH	1:A:1982:GLU:O	2.12	0.68
1:B:1408:LEU:HD12	1:B:1495:SER:HB2	1.74	0.68
1:D:415:ILE:HG21	1:D:432:GLY:N	2.09	0.68
1:B:1039:TYR:OH	1:B:1982:GLU:O	2.11	0.67
1:C:1678:PHE:CZ	1:C:1707:MET:HE1	2.28	0.67
1:B:1373:LYS:HG3	1:B:1412:ILE:HG21	1.77	0.67
1:C:1321:MET:HB3	1:C:1584:ILE:HG21	1.75	0.67
1:B:1907:ARG:NH1	1:C:158:GLU:OE1	2.28	0.67
1:D:226:VAL:HG21	1:D:879:VAL:HG11	1.76	0.67
1:A:750:ASN:HB3	1:A:754:THR:HG22	1.77	0.67
1:A:1827:THR:OG1	1:A:1893:GLN:NE2	2.27	0.66
1:C:346:TYR:HE1	1:C:359:ILE:HG22	1.60	0.66
1:E:343:ASN:HA	1:E:363:PHE:HB2	1.75	0.66
1:C:778:GLU:OE2	1:C:778:GLU:N	2.27	0.66
1:B:220:LEU:HG	1:B:227:MET:HG3	1.78	0.66
1:B:1485:GLY:HA2	1:B:1494:PHE:HD1	1.61	0.66
1:C:343:ASN:HA	1:C:363:PHE:HB2	1.76	0.66
1:C:226:VAL:HG21	1:C:879:VAL:HG11	1.78	0.66
1:D:977:VAL:HB	1:D:981:ILE:HD11	1.77	0.66
1:A:603:LEU:HD11	1:A:640:VAL:HG22	1.78	0.66
1:C:1689:THR:O	1:C:1724:ARG:NH2	2.29	0.66
1:C:204:GLU:OE2	1:C:241:ASN:ND2	2.24	0.66
1:B:2336:MET:HE3	1:C:2074:MET:HE1	1.78	0.65
1:C:1485:GLY:HA3	1:C:1494:PHE:H	1.61	0.65
1:B:1633:ARG:HH22	1:B:1649:LEU:HD21	1.61	0.65
1:E:1612:TYR:HB3	1:E:1654:LEU:HD22	1.79	0.65
1:A:415:ILE:HG21	1:A:432:GLY:N	2.11	0.65
1:C:2390:LEU:HD11	1:C:2522:LEU:HB3	1.78	0.65
1:B:373:LEU:HB2	1:B:416:TYR:HB3	1.79	0.65
1:E:1039:TYR:OH	1:E:1982:GLU:O	2.14	0.65
1:D:2400:SER:O	1:D:2416:ARG:NH2	2.30	0.65
1:A:1684:ASN:HB3	1:A:1719:MET:HB2	1.78	0.65
1:A:346:TYR:HE1	1:A:359:ILE:HG22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:PRO:HG2	1:D:959:VAL:HB	1.80	0.64
1:D:26:GLN:N	1:D:27:TYR:HB3	2.13	0.64
1:C:221:SER:OG	1:C:495:ARG:NH2	2.29	0.64
1:D:343:ASN:HA	1:D:363:PHE:HB2	1.80	0.64
1:D:1331:THR:HG21	1:D:1581:LEU:HD13	1.78	0.64
1:D:2030:MET:HE1	1:E:2279:LYS:HB3	1.79	0.64
1:E:2400:SER:O	1:E:2416:ARG:NH2	2.30	0.64
1:A:2400:SER:O	1:A:2416:ARG:NH2	2.31	0.64
1:E:226:VAL:HG21	1:E:879:VAL:HG11	1.79	0.64
1:E:1380:LEU:O	1:E:1388:GLN:NE2	2.31	0.64
1:B:2515:THR:N	1:B:2516:ASP:HB2	2.11	0.64
1:D:1684:ASN:HB3	1:D:1719:MET:HB2	1.79	0.64
1:A:1380:LEU:HD21	1:A:1463:ASN:HB3	1.80	0.63
1:E:346:TYR:HE1	1:E:359:ILE:HG22	1.63	0.63
1:B:956:PRO:HG2	1:B:959:VAL:HB	1.81	0.63
1:C:1373:LYS:NZ	1:C:1409:GLY:O	2.30	0.63
1:D:1612:TYR:HB3	1:D:1654:LEU:HD22	1.81	0.63
1:E:360:ARG:HH12	1:E:417:ALA:HB1	1.63	0.63
1:B:343:ASN:HA	1:B:363:PHE:HB2	1.78	0.63
1:E:600:LEU:HD21	1:E:628:THR:HG21	1.79	0.63
1:C:956:PRO:HG2	1:C:959:VAL:HB	1.80	0.63
1:E:1426:GLN:HB3	1:E:1462:LEU:HD22	1.80	0.63
1:C:489:THR:OG1	1:C:507:ASN:ND2	2.32	0.63
1:D:192:ARG:HG2	1:D:249:ILE:HD11	1.81	0.63
1:C:185:MET:HE1	1:C:942:LEU:HD11	1.81	0.62
1:C:360:ARG:NH1	1:C:362:ASN:OD1	2.32	0.62
1:E:1416:ASN:HB3	1:E:1421:TYR:HB2	1.81	0.62
1:A:209:VAL:HG22	1:A:926:LEU:HD11	1.81	0.62
1:E:554:THR:HG22	1:E:556:ALA:H	1.63	0.62
1:B:346:TYR:HE1	1:B:359:ILE:HG22	1.65	0.62
1:A:1744:TYR:HB2	1:A:1766:GLN:HG2	1.81	0.62
1:B:1474:SER:O	1:B:1478:LYS:NZ	2.23	0.62
1:C:415:ILE:HG21	1:C:432:GLY:N	2.14	0.62
1:A:170:LEU:O	1:A:174:THR:HG23	2.00	0.62
1:B:600:LEU:HD21	1:B:628:THR:HG21	1.81	0.62
1:D:373:LEU:HB2	1:D:416:TYR:HB3	1.82	0.62
1:A:360:ARG:HH21	1:A:390:LEU:HD13	1.65	0.62
1:C:2519:LYS:O	1:C:2523:GLU:HG3	2.00	0.62
1:D:1228:LEU:HD11	1:D:1245:VAL:HG13	1.82	0.62
1:A:2515:THR:N	1:A:2516:ASP:HB2	2.12	0.61
1:E:1437:ARG:HB2	1:E:1455:PRO:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:PRO:HG3	1:C:535:LYS:HE3	1.80	0.61
1:E:1430:MET:HG3	1:E:1494:PHE:HD1	1.66	0.61
1:B:1388:GLN:HE21	1:B:1416:ASN:HD22	1.48	0.61
1:D:1500:SER:OG	1:D:1501:GLY:N	2.30	0.61
1:D:2104:ARG:NH1	1:E:2249:GLU:OE1	2.33	0.61
1:A:221:SER:OG	1:A:495:ARG:NH2	2.34	0.61
1:A:2281:LEU:HG	1:A:2285:MET:HE2	1.83	0.61
1:C:1:MET:HB3	1:C:1564:ILE:HG23	1.82	0.61
1:C:1440:LEU:HB2	1:C:1452:PHE:HB2	1.81	0.61
1:C:1517:THR:HG23	1:C:1570:VAL:HB	1.83	0.61
1:D:1185:GLU:OE1	1:D:1185:GLU:N	2.33	0.61
1:E:1804:GLU:HA	1:E:1808:TYR:HB2	1.82	0.61
1:A:1531:ASP:OD1	1:A:1531:ASP:N	2.34	0.61
1:D:2411:ILE:HG22	1:D:2511:PHE:HB2	1.83	0.61
1:A:956:PRO:HG2	1:A:959:VAL:HB	1.82	0.61
1:D:346:TYR:HE1	1:D:359:ILE:HG22	1.66	0.61
1:E:2515:THR:N	1:E:2516:ASP:HB2	2.14	0.61
1:B:1899:ASP:OD1	1:B:1917:TYR:OH	2.16	0.61
1:B:353:GLY:O	1:B:354:ASN:ND2	2.33	0.61
1:E:181:SER:O	1:E:185:MET:HG2	2.01	0.61
1:B:1265:MET:HE2	1:B:1273:PHE:HD2	1.65	0.60
1:E:1633:ARG:HH22	1:E:1649:LEU:HD21	1.64	0.60
1:A:2046:SER:HB3	1:A:2306:MET:HE2	1.83	0.60
1:A:2485:MET:HE3	1:E:2488:PHE:HB2	1.81	0.60
1:B:1739:GLU:HG2	1:B:1777:LYS:HE3	1.81	0.60
1:C:600:LEU:HD21	1:C:628:THR:HG21	1.82	0.60
1:D:1412:ILE:HB	1:D:1425:VAL:HG12	1.83	0.60
1:C:192:ARG:HG2	1:C:249:ILE:HD11	1.84	0.60
1:B:1744:TYR:HB2	1:B:1766:GLN:HG2	1.83	0.60
1:B:415:ILE:HG21	1:B:432:GLY:N	2.16	0.60
1:E:415:ILE:HG12	1:E:431:GLY:HA3	1.83	0.60
1:E:504:GLN:HA	1:E:507:ASN:HD22	1.66	0.60
1:B:241:ASN:O	1:B:457:THR:OG1	2.20	0.60
1:B:1177:ALA:HB3	1:C:2176:PHE:HB2	1.84	0.60
1:B:2104:ARG:NH1	1:C:2249:GLU:OE2	2.34	0.60
1:C:1370:ILE:HA	1:C:1374:GLN:HG3	1.82	0.60
1:C:2515:THR:N	1:C:2516:ASP:HB2	2.13	0.60
1:E:307:SER:O	1:E:309:SER:N	2.35	0.60
1:A:220:LEU:HG	1:A:227:MET:HG3	1.82	0.60
1:A:415:ILE:HG12	1:A:431:GLY:HA3	1.82	0.60
1:A:1500:SER:OG	1:A:1501:GLY:N	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2119:SER:HB3	1:D:2237:MET:HE2	1.83	0.59
1:C:375:LYS:HE3	1:C:381:GLY:HA2	1.83	0.59
1:D:404:ILE:HD13	1:D:414:LYS:HD2	1.82	0.59
1:C:2439:VAL:HG22	1:C:2532:ILE:HG23	1.84	0.59
1:D:1689:THR:O	1:D:1724:ARG:NH2	2.36	0.59
1:D:1744:TYR:HB2	1:D:1766:GLN:HG2	1.84	0.59
1:A:11:ILE:HD11	1:A:41:LEU:HG	1.85	0.59
1:B:374:ARG:NH1	1:B:403:ASN:O	2.35	0.59
1:E:2455:ALA:HB3	1:E:2474:LEU:HB2	1.83	0.59
1:A:489:THR:OG1	1:A:507:ASN:ND2	2.36	0.59
1:D:603:LEU:HD21	1:D:640:VAL:HG22	1.83	0.59
1:D:1340:GLN:HB2	1:D:1355:HIS:HB2	1.85	0.59
1:A:901:ALA:O	1:A:902:LEU:HB2	2.03	0.59
1:A:247:TYR:CZ	1:A:898:TYR:HB3	2.38	0.59
1:A:1319:LEU:HD22	1:A:1588:LEU:HD13	1.85	0.59
1:D:2515:THR:HB	1:D:2516:ASP:OD2	2.03	0.59
1:E:1185:GLU:N	1:E:1185:GLU:OE1	2.35	0.59
1:A:1633:ARG:HH22	1:A:1649:LEU:HD21	1.68	0.59
1:D:169:LEU:O	1:D:173:ILE:HG12	2.03	0.59
1:B:1250:LYS:HD3	1:B:1296:THR:HG22	1.84	0.58
1:C:1443:VAL:HG13	1:C:1445:ASN:H	1.66	0.58
1:D:1899:ASP:OD1	1:D:1917:TYR:OH	2.21	0.58
1:E:1250:LYS:HD3	1:E:1296:THR:HG22	1.84	0.58
1:B:408:GLU:O	1:B:412:GLY:HA3	2.03	0.58
1:C:209:VAL:HG22	1:C:926:LEU:HD11	1.84	0.58
1:E:1636:THR:HG22	1:E:1637:GLY:H	1.67	0.58
1:A:1487:ASN:HB2	1:A:1492:GLN:HB2	1.83	0.58
1:C:732:PRO:HB3	1:C:763:VAL:HG21	1.85	0.58
1:C:2249:GLU:O	1:C:2253:MET:HG3	2.03	0.58
1:D:1795:ASN:O	1:D:1795:ASN:ND2	2.36	0.58
1:D:2402:ASN:ND2	1:D:2419:ASP:OD2	2.37	0.58
1:E:11:ILE:HD11	1:E:41:LEU:HG	1.85	0.58
1:B:1667:TYR:OH	1:B:1673:GLY:O	2.18	0.58
1:E:142:ARG:NH2	1:E:144:ASP:OD2	2.35	0.58
1:A:169:LEU:O	1:A:173:ILE:HG12	2.04	0.58
1:B:360:ARG:HH12	1:B:417:ALA:HB1	1.69	0.58
1:B:1500:SER:OG	1:B:1501:GLY:N	2.37	0.58
1:C:1039:TYR:OH	1:C:1982:GLU:O	2.14	0.58
1:B:83:ILE:HG23	1:B:1880:MET:HE1	1.86	0.57
1:B:886:MET:HE3	1:C:569:GLY:H	1.67	0.57
1:A:1177:ALA:HB3	1:B:2176:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PHE:HB2	1:D:398:SER:HB3	1.86	0.57
1:D:901:ALA:O	1:D:902:LEU:HB2	2.04	0.57
1:C:408:GLU:O	1:C:412:GLY:HA3	2.05	0.57
1:C:603:LEU:HD21	1:C:640:VAL:HG22	1.85	0.57
1:E:956:PRO:HG2	1:E:959:VAL:HB	1.85	0.57
1:A:1255:PHE:HB3	1:A:1281:LEU:HG	1.87	0.57
1:B:1321:MET:HE3	1:B:1584:ILE:HG22	1.87	0.57
1:C:1827:THR:HG1	1:C:1893:GLN:HE22	1.51	0.57
1:D:317:THR:HG22	1:D:330:TYR:CE2	2.39	0.57
1:D:337:THR:HG23	1:D:432:GLY:HA2	1.87	0.57
1:D:1039:TYR:OH	1:D:1982:GLU:O	2.15	0.57
1:B:209:VAL:HG22	1:B:926:LEU:HD11	1.85	0.57
1:B:1222:LYS:HB3	1:B:1225:THR:HG22	1.86	0.57
1:C:241:ASN:O	1:C:457:THR:OG1	2.22	0.57
1:C:373:LEU:O	1:C:416:TYR:HB2	2.04	0.57
1:A:2249:GLU:O	1:A:2253:MET:HG3	2.04	0.57
1:D:489:THR:OG1	1:D:507:ASN:ND2	2.37	0.57
1:E:2351:VAL:HA	1:E:2354:GLU:HG2	1.86	0.57
1:A:1899:ASP:OD1	1:A:1917:TYR:OH	2.22	0.57
1:B:2076:GLU:OE2	1:C:2282:TYR:OH	2.23	0.57
1:B:2509:LEU:HD23	1:B:2528:ILE:HD13	1.86	0.57
1:C:1250:LYS:HD3	1:C:1296:THR:HG22	1.85	0.57
1:C:1375:ILE:HA	1:C:1378:MET:HE2	1.86	0.57
1:C:2400:SER:O	1:C:2416:ARG:NH2	2.38	0.57
1:D:1760:HIS:HB2	1:D:1773:ILE:HB	1.86	0.57
1:E:297:LEU:O	1:E:316:SER:OG	2.19	0.57
1:E:1899:ASP:OD1	1:E:1917:TYR:OH	2.22	0.57
1:C:513:GLN:NE2	1:C:538:GLU:HG2	2.19	0.57
1:D:1315:VAL:HG22	1:D:1590:VAL:HG22	1.85	0.57
1:A:1485:GLY:HA3	1:A:1494:PHE:H	1.69	0.56
1:B:2357:GLU:HB3	1:B:2537:ARG:HD2	1.87	0.56
1:B:360:ARG:HE	1:B:362:ASN:CG	2.13	0.56
1:E:2439:VAL:HG22	1:E:2532:ILE:HG22	1.86	0.56
1:A:343:ASN:HA	1:A:363:PHE:HB2	1.85	0.56
1:A:600:LEU:HD21	1:A:628:THR:HG21	1.87	0.56
1:C:1145:LYS:NZ	1:C:1147:ASP:OD1	2.35	0.56
1:C:1148:THR:HG23	1:C:1150:VAL:HG23	1.87	0.56
1:D:2427:PRO:O	1:D:2434:ARG:NH2	2.38	0.56
1:E:530:PRO:O	1:E:562:ARG:NH2	2.31	0.56
1:E:1681:HIS:CD2	1:E:1691:ARG:HG2	2.40	0.56
1:E:1760:HIS:HB2	1:E:1773:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:829:ASP:OD1	1:D:832:ARG:NH2	2.37	0.56
1:E:901:ALA:O	1:E:902:LEU:HB2	2.06	0.56
1:A:2488:PHE:HB2	1:B:2485:MET:HE3	1.87	0.56
1:B:1570:VAL:HG22	1:B:1585:LYS:HG2	1.88	0.56
1:D:1255:PHE:HB3	1:D:1281:LEU:HG	1.87	0.56
1:E:1694:TYR:OH	1:E:1710:PHE:O	2.18	0.56
1:B:1417:LYS:NZ	1:B:1504:ASP:OD1	2.35	0.56
1:B:1426:GLN:HB3	1:B:1462:LEU:HD22	1.87	0.56
1:C:211:MET:HA	1:C:211:MET:HE3	1.88	0.56
1:D:750:ASN:HB3	1:D:754:THR:HG22	1.87	0.56
1:E:1331:THR:HG21	1:E:1581:LEU:HD22	1.86	0.56
1:A:530:PRO:O	1:A:562:ARG:NH2	2.32	0.56
1:A:2249:GLU:OE1	1:E:2104:ARG:NH1	2.39	0.56
1:B:155:MET:HG3	1:B:986:LEU:HD12	1.86	0.56
1:C:697:ARG:NH1	1:C:728:ASP:OD2	2.35	0.56
1:D:1100:VAL:HB	1:D:1593:VAL:HG22	1.88	0.56
1:D:1827:THR:OG1	1:D:1893:GLN:NE2	2.30	0.56
1:E:1255:PHE:HB3	1:E:1281:LEU:HG	1.87	0.56
1:C:347:PHE:CE2	1:C:415:ILE:HD11	2.41	0.56
1:C:373:LEU:HG	1:C:382:ILE:HD13	1.88	0.56
1:C:1319:LEU:HD22	1:C:1588:LEU:HD13	1.86	0.56
1:E:1485:GLY:HA2	1:E:1494:PHE:CD2	2.37	0.56
1:B:2093:GLU:OE1	1:C:2264:HIS:NE2	2.34	0.56
1:C:169:LEU:O	1:C:173:ILE:HG12	2.04	0.56
1:C:1804:GLU:HA	1:C:1808:TYR:HB2	1.88	0.56
1:E:209:VAL:HG22	1:E:926:LEU:HD11	1.88	0.56
1:A:561:MET:HG3	1:A:571:LEU:HD22	1.87	0.56
1:B:221:SER:OG	1:B:495:ARG:NH2	2.37	0.56
1:B:898:TYR:HE1	1:B:909:LEU:HD11	1.70	0.56
1:B:1424:SER:O	1:B:1463:ASN:HA	2.06	0.56
1:D:1416:ASN:HB3	1:D:1421:TYR:HB2	1.88	0.56
1:D:1927:GLU:OE2	1:D:1995:ARG:NH1	2.31	0.56
1:E:1319:LEU:HD11	1:E:1586:GLN:HG2	1.88	0.56
1:E:1408:LEU:HD23	1:E:1428:HIS:HB2	1.88	0.56
1:B:1694:TYR:OH	1:B:1710:PHE:O	2.22	0.55
1:E:236:LEU:HB2	1:E:487:PHE:HB2	1.87	0.55
1:E:1406:SER:OG	1:E:1430:MET:SD	2.63	0.55
1:A:1408:LEU:HD21	1:A:1430:MET:HG3	1.88	0.55
1:B:409:TYR:CE1	1:B:414:LYS:HD3	2.41	0.55
1:B:1485:GLY:HA2	1:B:1494:PHE:CD1	2.41	0.55
1:C:247:TYR:CZ	1:C:898:TYR:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:ALA:O	1:C:902:LEU:HB2	2.06	0.55
1:C:1694:TYR:OH	1:C:1710:PHE:O	2.19	0.55
1:D:1333:MET:HE3	1:D:1582:GLY:HA3	1.87	0.55
1:A:80:ARG:HA	1:A:83:ILE:HD12	1.88	0.55
1:B:1319:LEU:HD22	1:B:1588:LEU:HD13	1.88	0.55
1:D:1319:LEU:HD22	1:D:1588:LEU:HD13	1.88	0.55
1:D:2509:LEU:HD23	1:D:2528:ILE:HD13	1.87	0.55
1:A:899:VAL:O	1:A:900:THR:OG1	2.25	0.55
1:A:1416:ASN:HB3	1:A:1421:TYR:HB2	1.87	0.55
1:A:2402:ASN:ND2	1:A:2419:ASP:OD2	2.35	0.55
1:D:223:ASN:ND2	1:D:878:ASP:OD2	2.39	0.55
1:E:1517:THR:HG23	1:E:1570:VAL:HB	1.87	0.55
1:C:1369:VAL:HG21	1:C:1399:VAL:HB	1.88	0.55
1:D:209:VAL:HG22	1:D:926:LEU:HD11	1.89	0.55
1:D:735:LEU:HD11	1:D:743:LEU:HD12	1.88	0.55
1:B:2219:ARG:HD3	1:B:2223:TRP:CH2	2.42	0.55
1:E:2406:LEU:HG	1:E:2411:ILE:HG12	1.87	0.55
1:A:1321:MET:HE3	1:A:1584:ILE:HG22	1.89	0.55
1:B:2249:GLU:O	1:B:2253:MET:HG3	2.06	0.55
1:D:1177:ALA:HB3	1:E:2176:PHE:HB2	1.89	0.55
1:E:1340:GLN:HB3	1:E:1355:HIS:HB2	1.89	0.55
1:E:1518:VAL:HG21	1:E:1553:ILE:HG12	1.88	0.55
1:A:1483:VAL:HG13	1:A:1493:ILE:HG23	1.88	0.55
1:A:1804:GLU:HA	1:A:1808:TYR:HB2	1.88	0.55
1:B:236:LEU:HB2	1:B:487:PHE:HB2	1.89	0.55
1:B:2104:ARG:NH2	1:B:2107:ASP:OD2	2.35	0.55
1:D:1536:LEU:HD23	1:D:1537:PRO:HD2	1.88	0.55
1:D:2219:ARG:HD3	1:D:2223:TRP:CH2	2.42	0.55
1:A:1443:VAL:HG13	1:A:1445:ASN:H	1.72	0.55
1:C:1899:ASP:OD1	1:C:1917:TYR:OH	2.24	0.55
1:A:2129:LYS:NZ	1:B:2228:ASP:OD2	2.40	0.55
1:B:169:LEU:O	1:B:173:ILE:HG12	2.07	0.55
1:B:1738:TRP:HZ2	1:B:1770:VAL:HG11	1.72	0.55
1:A:315:ILE:HG22	1:A:332:ILE:HB	1.89	0.54
1:D:11:ILE:HD11	1:D:41:LEU:HG	1.88	0.54
1:D:692:ALA:HA	1:D:741:MET:HE3	1.88	0.54
1:E:2390:LEU:HD11	1:E:2522:LEU:HB3	1.88	0.54
1:B:80:ARG:HA	1:B:83:ILE:HG12	1.89	0.54
1:B:142:ARG:NH2	1:B:144:ASP:OD2	2.32	0.54
1:E:642:TRP:HZ2	1:E:804:ILE:HG21	1.72	0.54
1:A:732:PRO:HB3	1:A:763:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2282:TYR:OH	1:E:2076:GLU:OE2	2.23	0.54
1:B:1255:PHE:HB3	1:B:1281:LEU:HG	1.90	0.54
1:C:80:ARG:HA	1:C:83:ILE:HG12	1.89	0.54
1:C:307:SER:O	1:C:309:SER:N	2.40	0.54
1:A:1100:VAL:HB	1:A:1593:VAL:HG22	1.89	0.54
1:A:1601:LEU:HD23	1:A:1615:LEU:HB2	1.88	0.54
1:A:2093:GLU:OE1	1:B:2264:HIS:NE2	2.36	0.54
1:D:181:SER:O	1:D:185:MET:HG2	2.07	0.54
1:D:1150:VAL:HG11	1:D:1157:ILE:HD12	1.88	0.54
1:E:347:PHE:CZ	1:E:415:ILE:HD11	2.43	0.54
1:B:192:ARG:HG2	1:B:249:ILE:HD11	1.90	0.54
1:A:236:LEU:HB2	1:A:487:PHE:HB2	1.90	0.54
1:A:247:TYR:OH	1:A:480:ASP:OD1	2.25	0.54
1:B:91:SER:HB3	1:B:1960:LEU:HD11	1.88	0.54
1:B:2453:ILE:HG23	1:B:2521:LEU:HD21	1.90	0.54
1:C:1408:LEU:HD21	1:C:1430:MET:HG2	1.89	0.54
1:A:697:ARG:NH1	1:A:728:ASP:OD2	2.36	0.54
1:B:307:SER:O	1:B:309:SER:N	2.41	0.54
1:E:1100:VAL:HB	1:E:1593:VAL:HG22	1.89	0.54
1:A:504:GLN:HA	1:A:507:ASN:ND2	2.23	0.54
1:B:901:ALA:O	1:B:902:LEU:HB2	2.07	0.54
1:C:1633:ARG:HH22	1:C:1649:LEU:HD21	1.71	0.54
1:D:2076:GLU:OE2	1:E:2282:TYR:OH	2.26	0.54
1:E:1509:ILE:HG12	1:E:1514:ILE:HD11	1.90	0.54
1:A:1265:MET:HE2	1:A:1273:PHE:CD2	2.43	0.54
1:A:1369:VAL:HG11	1:A:1399:VAL:HB	1.90	0.54
1:C:1235:PHE:HB3	1:C:1240:THR:HG22	1.88	0.54
1:C:2427:PRO:O	1:C:2434:ARG:NH2	2.40	0.54
1:B:1807:TYR:O	1:B:1811:MET:HG2	2.08	0.53
1:B:2519:LYS:O	1:B:2523:GLU:HG3	2.08	0.53
1:D:1738:TRP:HE3	1:D:1756:ASN:HD22	1.54	0.53
1:D:2057:THR:O	1:D:2061:VAL:HG23	2.08	0.53
1:E:1319:LEU:HD22	1:E:1588:LEU:HD13	1.90	0.53
1:B:621:SER:O	1:B:624:ASN:ND2	2.41	0.53
1:D:551:GLU:HG2	1:D:552:GLN:HG2	1.90	0.53
1:D:1405:TYR:OH	1:D:1492:GLN:OE1	2.15	0.53
1:D:2453:ILE:HG23	1:D:2521:LEU:HD21	1.90	0.53
1:E:365:VAL:HG13	1:E:367:ARG:HH21	1.73	0.53
1:E:404:ILE:HD13	1:E:414:LYS:HD2	1.90	0.53
1:E:732:PRO:HB3	1:E:763:VAL:HG21	1.90	0.53
1:C:616:MET:HE2	1:C:661:TRP:CG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1714:ALA:HB3	1:C:1717:TYR:HB2	1.90	0.53
1:E:1372:ASN:C	1:E:1373:LYS:HD3	2.32	0.53
1:A:554:THR:HG22	1:A:556:ALA:H	1.72	0.53
1:C:315:ILE:HG22	1:C:332:ILE:HB	1.89	0.53
1:B:1374:GLN:O	1:B:1378:MET:HG3	2.08	0.53
1:C:1401:HIS:NE2	1:C:1403:GLY:O	2.41	0.53
1:D:221:SER:OG	1:D:495:ARG:NH2	2.39	0.53
1:E:501:ASP:O	1:E:505:VAL:HG23	2.09	0.53
1:A:307:SER:O	1:A:309:SER:N	2.42	0.53
1:C:735:LEU:HD11	1:C:743:LEU:HD12	1.90	0.53
1:D:1436:ARG:HG2	1:D:1494:PHE:HE2	1.72	0.53
1:C:372:THR:HA	1:C:416:TYR:O	2.08	0.53
1:E:690:ASP:OD2	1:E:691:MET:N	2.41	0.53
1:A:829:ASP:OD1	1:A:832:ARG:NH2	2.39	0.53
1:A:2076:GLU:OE2	1:B:2282:TYR:OH	2.26	0.53
1:C:360:ARG:HD2	1:C:386:LEU:HD13	1.91	0.53
1:A:192:ARG:HG2	1:A:249:ILE:HD11	1.90	0.53
1:C:11:ILE:HD11	1:C:41:LEU:HG	1.90	0.53
1:C:347:PHE:CE1	1:C:360:ARG:HG3	2.44	0.53
1:D:2249:GLU:O	1:D:2253:MET:HG3	2.10	0.53
1:E:247:TYR:CZ	1:E:898:TYR:HB3	2.44	0.53
1:A:1694:TYR:OH	1:A:1710:PHE:O	2.24	0.52
1:B:1664:LEU:HD21	1:B:1727:VAL:HG21	1.91	0.52
1:B:2282:TYR:O	1:B:2286:ARG:HG2	2.08	0.52
1:D:1319:LEU:HD11	1:D:1586:GLN:HG2	1.90	0.52
1:A:2427:PRO:O	1:A:2434:ARG:NH2	2.41	0.52
1:D:600:LEU:HD21	1:D:628:THR:HG21	1.90	0.52
1:D:2129:LYS:NZ	1:E:2228:ASP:OD2	2.43	0.52
1:E:408:GLU:O	1:E:412:GLY:HA3	2.10	0.52
1:E:603:LEU:HD21	1:E:640:VAL:HG22	1.92	0.52
1:E:1510:ASN:O	1:E:1514:ILE:HD12	2.10	0.52
1:A:317:THR:HG22	1:A:330:TYR:CE2	2.45	0.52
1:B:1804:GLU:HA	1:B:1808:TYR:HB2	1.91	0.52
1:C:2030:MET:HE1	1:D:2279:LYS:HB3	1.92	0.52
1:C:2219:ARG:HD3	1:C:2223:TRP:CH2	2.45	0.52
1:E:1803:TRP:CZ2	1:E:1854:PRO:HB2	2.44	0.52
1:A:1437:ARG:HB3	1:A:1455:PRO:HA	1.92	0.52
1:B:1921:LEU:HD13	1:B:1994:LEU:HD13	1.92	0.52
1:C:236:LEU:HB2	1:C:487:PHE:HB2	1.91	0.52
1:B:11:ILE:HD11	1:B:41:LEU:HG	1.92	0.52
1:B:697:ARG:NH1	1:B:728:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2129:LYS:NZ	1:C:2228:ASP:OD2	2.43	0.52
1:D:236:LEU:HB2	1:D:487:PHE:HB2	1.91	0.52
1:D:347:PHE:HE2	1:D:417:ALA:HB2	1.75	0.52
1:D:697:ARG:NH1	1:D:728:ASP:OD2	2.36	0.52
1:B:2137:ASP:O	1:C:2218:ARG:NH2	2.42	0.52
1:C:117:GLY:O	1:C:121:GLU:HG2	2.10	0.52
1:D:1373:LYS:HB3	1:D:1412:ILE:HG13	1.91	0.52
1:E:169:LEU:O	1:E:173:ILE:HG12	2.09	0.52
1:E:349:LEU:HD11	1:E:356:GLN:HB3	1.91	0.52
1:B:22:LEU:HD21	1:B:52:GLU:HB3	1.91	0.52
1:B:63:LEU:HD11	1:B:88:VAL:HG21	1.91	0.52
1:B:347:PHE:CE1	1:B:415:ILE:HD11	2.45	0.52
1:B:561:MET:HG3	1:B:571:LEU:HD22	1.91	0.52
1:B:2277:THR:HA	1:B:2281:LEU:HD23	1.90	0.52
1:D:365:VAL:HG22	1:D:392:ALA:H	1.75	0.52
1:B:247:TYR:CZ	1:B:898:TYR:HB3	2.45	0.52
1:B:1531:ASP:OD1	1:B:1531:ASP:N	2.42	0.52
1:B:1922:GLU:HB3	1:C:1004:ILE:HD13	1.92	0.52
1:C:1485:GLY:CA	1:C:1494:PHE:H	2.23	0.52
1:C:1744:TYR:HB2	1:C:1766:GLN:HG2	1.92	0.52
1:E:1265:MET:HE2	1:E:1273:PHE:CD2	2.44	0.52
1:E:1400:LYS:H	1:E:1498:GLN:HG2	1.75	0.52
1:A:1252:TYR:O	1:A:1288:LYS:NZ	2.37	0.52
1:A:1319:LEU:HD11	1:A:1586:GLN:HG2	1.92	0.52
1:B:83:ILE:HD12	1:B:1880:MET:HE1	1.90	0.52
1:B:1036:LEU:HD11	1:B:1871:PRO:HD3	1.92	0.52
1:C:473:ASN:ND2	1:C:477:ILE:HG12	2.25	0.52
1:C:2509:LEU:HD23	1:C:2528:ILE:HD13	1.92	0.52
1:D:373:LEU:HD22	1:D:382:ILE:HD13	1.92	0.52
1:D:504:GLN:HA	1:D:507:ASN:ND2	2.25	0.52
1:E:221:SER:OG	1:E:495:ARG:NH2	2.39	0.52
1:A:346:TYR:OH	1:A:395:ASN:OD1	2.20	0.51
1:A:893:LEU:HD23	1:A:918:LEU:HD21	1.93	0.51
1:A:2134:TYR:CE1	1:A:2224:GLU:HB2	2.44	0.51
1:A:2410:GLN:NE2	1:A:2412:GLU:OE2	2.42	0.51
1:B:732:PRO:HB3	1:B:763:VAL:HG21	1.91	0.51
1:C:2076:GLU:OE2	1:D:2282:TYR:OH	2.27	0.51
1:D:556:ALA:HB1	1:D:589:LEU:HD11	1.92	0.51
1:E:538:GLU:HG3	1:E:591:VAL:HG22	1.91	0.51
1:A:1300:ASP:OD2	1:A:1604:ARG:NH2	2.35	0.51
1:B:415:ILE:HG12	1:B:431:GLY:CA	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ALA:HB1	1:B:589:LEU:HD11	1.92	0.51
1:B:1673:GLY:HA3	1:B:1731:LYS:HE2	1.92	0.51
1:B:1827:THR:HG1	1:B:1893:GLN:HE22	1.54	0.51
1:B:2350:LYS:HD2	1:C:2299:LEU:HD22	1.91	0.51
1:C:582:ASP:OD2	1:C:583:ALA:N	2.41	0.51
1:E:373:LEU:HG	1:E:382:ILE:HD13	1.92	0.51
1:D:1677:TRP:CZ2	1:D:1730:GLN:HB2	2.46	0.51
1:A:505:VAL:HG11	1:A:598:TYR:HD2	1.76	0.51
1:B:2314:GLU:OE2	1:B:2352:TRP:NE1	2.39	0.51
1:A:1636:THR:HG22	1:A:1637:GLY:H	1.75	0.51
1:B:620:LEU:HD22	1:B:664:CYS:HB3	1.93	0.51
1:D:732:PRO:HB3	1:D:763:VAL:HG21	1.91	0.51
1:C:1827:THR:OG1	1:C:1893:GLN:NE2	2.28	0.51
1:A:1738:TRP:HE3	1:A:1756:ASN:HD22	1.57	0.51
1:B:1636:THR:HG22	1:B:1637:GLY:H	1.76	0.51
1:C:358:PHE:HB2	1:C:398:SER:OG	2.11	0.51
1:D:1435:THR:HG22	1:D:1437:ARG:HD3	1.92	0.51
1:E:373:LEU:HB2	1:E:416:TYR:HB3	1.92	0.51
1:E:1744:TYR:HB2	1:E:1766:GLN:OE1	2.11	0.51
1:A:1004:ILE:HD13	1:E:1922:GLU:HB3	1.92	0.51
1:A:2057:THR:O	1:A:2061:VAL:HG23	2.10	0.51
1:B:1519:MET:HE3	1:B:1568:ASP:HB3	1.93	0.51
1:B:1803:TRP:CZ2	1:B:1854:PRO:HB2	2.46	0.51
1:C:170:LEU:O	1:C:174:THR:HG23	2.10	0.51
1:C:1108:TRP:CE2	1:C:1161:ILE:HD11	2.46	0.51
1:E:220:LEU:HG	1:E:227:MET:HG3	1.93	0.51
1:E:360:ARG:HE	1:E:362:ASN:CG	2.19	0.51
1:E:1458:PRO:HB2	1:E:1461:ILE:HB	1.92	0.51
1:E:2119:SER:HB3	1:E:2237:MET:HE2	1.91	0.51
1:A:241:ASN:O	1:A:457:THR:OG1	2.28	0.51
1:A:271:ILE:HD13	1:A:281:TRP:HZ2	1.75	0.51
1:A:2509:LEU:HD23	1:A:2528:ILE:HD13	1.93	0.51
1:C:1440:LEU:HB3	1:C:1479:CYS:HB3	1.92	0.51
1:D:1321:MET:HE3	1:D:1584:ILE:HG22	1.91	0.51
1:E:2411:ILE:HD12	1:E:2522:LEU:HD23	1.93	0.51
1:A:257:LYS:HD3	1:A:257:LYS:N	2.25	0.51
1:A:408:GLU:O	1:A:412:GLY:HA3	2.10	0.51
1:B:216:THR:HG22	1:B:494:HIS:HB3	1.91	0.51
1:B:1340:GLN:HB2	1:B:1355:HIS:HB2	1.93	0.51
1:D:307:SER:O	1:D:309:SER:N	2.44	0.51
1:D:680:LEU:HD11	1:D:757:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2218:ARG:O	1:D:2222:GLU:HG2	2.11	0.51
1:D:2311:LEU:HD22	1:D:2348:MET:HG2	1.93	0.51
1:E:241:ASN:O	1:E:457:THR:OG1	2.29	0.51
1:E:2249:GLU:O	1:E:2253:MET:HG3	2.11	0.51
1:A:349:LEU:HD11	1:A:356:GLN:HB3	1.91	0.50
1:C:367:ARG:HD2	1:C:367:ARG:N	2.26	0.50
1:E:315:ILE:HG22	1:E:332:ILE:HB	1.93	0.50
1:E:1235:PHE:HB3	1:E:1240:THR:HG22	1.93	0.50
1:B:510:VAL:HB	1:B:591:VAL:HG12	1.93	0.50
1:B:750:ASN:HB3	1:B:754:THR:HG22	1.94	0.50
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.93	0.50
1:C:1340:GLN:HB2	1:C:1355:HIS:HB2	1.93	0.50
1:B:358:PHE:HB2	1:B:398:SER:HB3	1.93	0.50
1:B:1235:PHE:HB3	1:B:1240:THR:HG23	1.93	0.50
1:C:893:LEU:HD23	1:C:918:LEU:HD21	1.92	0.50
1:E:26:GLN:N	1:E:27:TYR:HB3	2.26	0.50
1:E:2053:MET:HE2	1:E:2306:MET:CG	2.41	0.50
1:B:1870:ASP:HB3	1:B:1873:ALA:HB3	1.93	0.50
1:C:2057:THR:O	1:C:2061:VAL:HG23	2.11	0.50
1:D:142:ARG:NH2	1:D:144:ASP:OD2	2.36	0.50
1:D:241:ASN:O	1:D:457:THR:OG1	2.28	0.50
1:E:347:PHE:CE2	1:E:415:ILE:HD11	2.45	0.50
1:A:80:ARG:HD3	1:A:83:ILE:HD12	1.93	0.50
1:A:735:LEU:HD11	1:A:743:LEU:HD12	1.94	0.50
1:C:1416:ASN:HB3	1:C:1421:TYR:HB2	1.92	0.50
1:B:1319:LEU:HD11	1:B:1586:GLN:HG2	1.93	0.50
1:B:1415:TYR:CE2	1:B:1473:THR:HG22	2.47	0.50
1:D:1647:GLN:HA	1:D:1792:MET:HE2	1.94	0.50
1:D:2342:LEU:HD13	1:E:2063:GLN:NE2	2.27	0.50
1:A:1457:SER:HB3	1:A:1458:PRO:CD	2.41	0.50
1:A:1677:TRP:CZ2	1:A:1730:GLN:HB2	2.46	0.50
1:B:735:LEU:HD11	1:B:743:LEU:HD12	1.94	0.50
1:C:899:VAL:O	1:C:899:VAL:HG12	2.12	0.50
1:D:197:THR:O	1:D:453:ARG:NH1	2.45	0.50
1:A:1049:ARG:HH21	1:A:1056:MET:HE2	1.77	0.50
1:A:1264:GLY:HA3	1:A:1276:MET:HE3	1.94	0.50
1:B:1408:LEU:HD21	1:B:1430:MET:HG2	1.94	0.50
1:B:2439:VAL:HG22	1:B:2532:ILE:HG22	1.93	0.50
1:D:63:LEU:HD11	1:D:88:VAL:HG21	1.94	0.50
1:D:271:ILE:HD13	1:D:281:TRP:HZ2	1.77	0.50
1:D:1383:VAL:HG12	1:D:1421:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1760:HIS:HB2	1:A:1773:ILE:HB	1.93	0.50
1:A:2219:ARG:HD3	1:A:2223:TRP:CH2	2.47	0.50
1:D:1419:LYS:HB3	1:D:1421:TYR:CE1	2.47	0.50
1:E:1412:ILE:O	1:E:1424:SER:HA	2.12	0.50
1:A:1293:ILE:HG13	1:A:1302:VAL:HG23	1.94	0.49
1:B:2336:MET:CE	1:C:2074:MET:HE1	2.41	0.49
1:C:1228:LEU:HD11	1:C:1245:VAL:HG13	1.93	0.49
1:C:1400:LYS:H	1:C:1498:GLN:HG2	1.77	0.49
1:E:893:LEU:HD23	1:E:918:LEU:HD21	1.94	0.49
1:C:347:PHE:CD2	1:C:415:ILE:HD11	2.47	0.49
1:C:687:ILE:HD11	1:C:741:MET:HE2	1.94	0.49
1:A:783:VAL:HG13	1:A:832:ARG:HG3	1.95	0.49
1:E:531:PRO:HG3	1:E:535:LYS:NZ	2.27	0.49
1:B:505:VAL:HG11	1:B:598:TYR:HD2	1.76	0.49
1:C:26:GLN:N	1:C:27:TYR:HB3	2.26	0.49
1:C:530:PRO:O	1:C:562:ARG:NH2	2.25	0.49
1:C:1265:MET:HE2	1:C:1273:PHE:CD2	2.47	0.49
1:D:1458:PRO:HD2	1:D:1461:ILE:HG21	1.93	0.49
1:D:1636:THR:HG22	1:D:1637:GLY:H	1.76	0.49
1:D:1694:TYR:OH	1:D:1710:PHE:O	2.24	0.49
1:E:2427:PRO:O	1:E:2434:ARG:NH2	2.44	0.49
1:A:1010:ALA:O	1:A:1014:THR:HG23	2.13	0.49
1:B:1677:TRP:CZ2	1:B:1730:GLN:HB2	2.48	0.49
1:C:1150:VAL:HG11	1:C:1157:ILE:HD12	1.94	0.49
1:D:1130:MET:HE3	1:D:1133:GLY:HA2	1.94	0.49
1:E:1150:VAL:HG11	1:E:1157:ILE:HD12	1.94	0.49
1:E:2057:THR:O	1:E:2061:VAL:HG23	2.12	0.49
1:A:1480:SER:OG	1:A:1481:TYR:N	2.45	0.49
1:B:899:VAL:O	1:B:900:THR:OG1	2.26	0.49
1:B:1477:LYS:HB2	1:B:1478:LYS:HZ2	1.77	0.49
1:D:2275:LYS:O	1:D:2278:ASN:ND2	2.45	0.49
1:E:1673:GLY:HA3	1:E:1731:LYS:HE2	1.94	0.49
1:A:1235:PHE:HB3	1:A:1240:THR:HG22	1.94	0.49
1:A:1265:MET:HE2	1:A:1273:PHE:HD2	1.78	0.49
1:A:1302:VAL:HG12	1:A:1604:ARG:HG2	1.94	0.49
1:B:323:ASN:HD21	1:B:354:ASN:HD21	1.60	0.49
1:B:1116:ASN:HB2	1:C:1207:TRP:CD1	2.48	0.49
1:B:1441:THR:HB	1:B:1450:ARG:HA	1.94	0.49
1:B:1135:LEU:HD12	1:B:1620:ILE:HD13	1.94	0.49
1:C:63:LEU:HD11	1:C:88:VAL:HG21	1.94	0.49
1:C:1417:LYS:NZ	1:C:1504:ASP:OD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2368:LEU:HD12	1:D:2528:ILE:HB	1.93	0.49
1:E:1126:ASP:OD1	1:E:1128:SER:OG	2.21	0.49
1:B:415:ILE:HG21	1:B:432:GLY:H	1.77	0.49
1:C:1518:VAL:HG21	1:C:1553:ILE:HG12	1.95	0.49
1:C:1636:THR:HG22	1:C:1637:GLY:H	1.78	0.49
1:E:1408:LEU:HD21	1:E:1430:MET:HG2	1.95	0.49
1:E:2134:TYR:CE1	1:E:2224:GLU:HB2	2.48	0.49
1:A:91:SER:HB3	1:A:1960:LEU:HD11	1.95	0.49
1:B:1150:VAL:HG11	1:B:1157:ILE:HD12	1.95	0.49
1:C:349:LEU:HD11	1:C:356:GLN:HB3	1.95	0.49
1:C:616:MET:HE2	1:C:661:TRP:CD2	2.48	0.49
1:D:1302:VAL:HG12	1:D:1604:ARG:HG2	1.94	0.49
1:E:1265:MET:HE2	1:E:1273:PHE:HD2	1.78	0.49
1:A:158:GLU:CD	1:E:1907:ARG:HH12	2.20	0.48
1:B:337:THR:HA	1:B:537:PHE:CE2	2.48	0.48
1:B:603:LEU:HD21	1:B:640:VAL:HG22	1.95	0.48
1:B:829:ASP:OD1	1:B:832:ARG:NH2	2.45	0.48
1:B:1409:GLY:HA3	1:B:1427:GLY:H	1.77	0.48
1:B:2057:THR:O	1:B:2061:VAL:HG23	2.13	0.48
1:C:1302:VAL:HG12	1:C:1604:ARG:HG2	1.95	0.48
1:C:1736:ASN:HB2	1:C:1739:GLU:CD	2.38	0.48
1:A:367:ARG:N	1:A:367:ARG:HD2	2.27	0.48
1:A:556:ALA:HB1	1:A:589:LEU:HD11	1.94	0.48
1:A:1460:THR:HG23	1:A:1460:THR:O	2.13	0.48
1:B:1972:ALA:O	1:B:1974:SER:N	2.45	0.48
1:C:420:TYR:CD2	1:C:426:ALA:HB2	2.49	0.48
1:E:200:HIS:HB3	1:E:203:TYR:HB3	1.95	0.48
1:A:1570:VAL:HG22	1:A:1585:LYS:HG2	1.94	0.48
1:B:530:PRO:O	1:B:562:ARG:NH2	2.34	0.48
1:B:1010:ALA:O	1:B:1014:THR:HG23	2.13	0.48
1:C:556:ALA:HB1	1:C:589:LEU:HD11	1.95	0.48
1:C:1907:ARG:HH22	1:D:158:GLU:CD	2.20	0.48
1:D:704:LEU:HD11	1:D:741:MET:HG3	1.94	0.48
1:E:337:THR:HA	1:E:537:PHE:CE2	2.48	0.48
1:E:1383:VAL:H	1:E:1421:TYR:HE2	1.61	0.48
1:C:2453:ILE:O	1:C:2475:SER:HA	2.12	0.48
1:D:409:TYR:CE1	1:D:414:LYS:HD3	2.48	0.48
1:D:902:LEU:O	1:D:903:ASN:HB2	2.12	0.48
1:E:1036:LEU:HD11	1:E:1871:PRO:HD3	1.95	0.48
1:B:2416:ARG:NH1	1:B:2504:SER:O	2.46	0.48
1:C:411:ASN:H	1:C:435:THR:HG23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:GLN:O	1:C:1816:ARG:NH2	2.47	0.48
1:D:1436:ARG:HG2	1:D:1494:PHE:CE2	2.48	0.48
1:D:2212:ARG:NH1	1:E:2211:SER:OG	2.46	0.48
1:E:1827:THR:OG1	1:E:1893:GLN:NE2	2.29	0.48
1:A:1331:THR:HG21	1:A:1581:LEU:HD13	1.96	0.48
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.96	0.48
1:D:1485:GLY:HA2	1:D:1494:PHE:H	1.78	0.48
1:E:862:ASN:OD1	1:E:862:ASN:N	2.43	0.48
1:E:902:LEU:O	1:E:903:ASN:HB2	2.14	0.48
1:A:680:LEU:HD11	1:A:757:LEU:HD21	1.95	0.48
1:B:795:LYS:O	1:B:797:GLN:HG2	2.13	0.48
1:B:1426:GLN:NE2	1:B:1428:HIS:O	2.44	0.48
1:C:1510:ASN:O	1:C:1514:ILE:HD12	2.13	0.48
1:E:1921:LEU:HD13	1:E:1994:LEU:HD13	1.96	0.48
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.95	0.48
1:A:337:THR:HA	1:A:537:PHE:CE2	2.48	0.48
1:B:1265:MET:HE2	1:B:1273:PHE:CD2	2.48	0.48
1:C:1036:LEU:HD11	1:C:1871:PRO:HD3	1.94	0.48
1:E:513:GLN:NE2	1:E:538:GLU:OE1	2.41	0.48
1:E:829:ASP:OD1	1:E:832:ARG:NH2	2.46	0.48
1:E:1744:TYR:CE1	1:E:1753:VAL:HB	2.49	0.48
1:A:2253:MET:HE3	1:E:2101:ILE:HG12	1.96	0.48
1:B:1738:TRP:HE3	1:B:1756:ASN:HD22	1.61	0.48
1:B:2030:MET:HE1	1:C:2279:LYS:HB3	1.95	0.48
1:C:2515:THR:H	1:C:2516:ASP:CB	2.19	0.48
1:D:1293:ILE:HG13	1:D:1302:VAL:HG23	1.96	0.48
1:E:1478:LYS:HA	1:E:1478:LYS:HD3	1.77	0.48
1:E:1793:ASP:HB3	1:E:1796:SER:HB3	1.94	0.48
1:A:409:TYR:CE1	1:A:414:LYS:HD3	2.49	0.48
1:A:620:LEU:HD22	1:A:664:CYS:HB3	1.96	0.48
1:B:117:GLY:O	1:B:121:GLU:HG2	2.14	0.48
1:C:1010:ALA:O	1:C:1014:THR:HG23	2.14	0.48
1:C:1792:MET:O	1:C:1853:ARG:NH1	2.36	0.48
1:D:899:VAL:O	1:D:900:THR:OG1	2.25	0.48
1:D:1633:ARG:HH22	1:D:1649:LEU:HD21	1.79	0.48
1:D:2455:ALA:HB3	1:D:2474:LEU:HB2	1.95	0.48
1:A:1601:LEU:HD22	1:A:1613:MET:SD	2.53	0.47
1:C:247:TYR:OH	1:C:480:ASP:OD1	2.25	0.47
1:C:2277:THR:HA	1:C:2281:LEU:HD23	1.96	0.47
1:E:510:VAL:HB	1:E:591:VAL:HG12	1.95	0.47
1:E:1252:TYR:O	1:E:1288:LYS:NZ	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2455:ALA:HB1	1:E:2509:LEU:HD11	1.95	0.47
1:A:365:VAL:HG13	1:A:391:ILE:HA	1.95	0.47
1:B:26:GLN:N	1:B:27:TYR:HB3	2.29	0.47
1:C:2104:ARG:HD3	1:C:2104:ARG:HA	1.65	0.47
1:B:360:ARG:HD2	1:B:386:LEU:HD13	1.96	0.47
1:B:2191:ALA:O	1:B:2195:VAL:HG13	2.14	0.47
1:C:510:VAL:HB	1:C:591:VAL:HG12	1.96	0.47
1:C:1540:SER:O	1:C:1544:MET:HE2	2.14	0.47
1:E:1972:ALA:O	1:E:1975:LEU:N	2.42	0.47
1:A:852:VAL:O	1:A:856:MET:HG3	2.14	0.47
1:B:1308:ARG:O	1:B:1595:TYR:OH	2.30	0.47
1:B:1514:ILE:HG12	1:B:1573:THR:HG23	1.96	0.47
1:C:1293:ILE:HG13	1:C:1302:VAL:HG23	1.96	0.47
1:C:1457:SER:OG	1:C:1458:PRO:HD3	2.14	0.47
1:C:1972:ALA:O	1:C:1975:LEU:HG	2.14	0.47
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.78	0.47
1:D:349:LEU:HD11	1:D:356:GLN:HB3	1.95	0.47
1:E:2219:ARG:HD3	1:E:2223:TRP:CH2	2.49	0.47
1:A:1443:VAL:HG11	1:A:1446:ASN:HB3	1.96	0.47
1:B:1515:LYS:HB3	1:B:1528:THR:HG22	1.97	0.47
1:B:1724:ARG:HG2	1:B:1742:PHE:CZ	2.49	0.47
1:E:347:PHE:HE2	1:E:417:ALA:HB2	1.79	0.47
1:E:538:GLU:OE2	1:E:538:GLU:N	2.45	0.47
1:E:540:ASP:HB3	1:E:542:ASN:OD1	2.13	0.47
1:E:1300:ASP:OD2	1:E:1604:ARG:NH2	2.36	0.47
1:A:337:THR:N	1:A:431:GLY:O	2.37	0.47
1:A:960:SER:HB3	1:A:1400:LYS:HD2	1.96	0.47
1:A:1250:LYS:HD3	1:A:1296:THR:HG22	1.96	0.47
1:B:2074:MET:SD	1:B:2285:MET:HE3	2.54	0.47
1:B:2134:TYR:CE1	1:B:2224:GLU:HB2	2.50	0.47
1:C:473:ASN:HD21	1:C:477:ILE:H	1.61	0.47
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.62	0.47
1:A:2519:LYS:O	1:A:2523:GLU:HG3	2.14	0.47
1:B:977:VAL:HB	1:B:981:ILE:HD11	1.96	0.47
1:B:1503:LEU:HD12	1:B:1504:ASP:H	1.80	0.47
1:B:1536:LEU:HD13	1:B:1537:PRO:HD2	1.97	0.47
1:B:1914:LYS:NZ	1:C:974:ASP:OD2	2.37	0.47
1:C:215:SER:O	1:C:216:THR:OG1	2.27	0.47
1:C:1720:HIS:O	1:C:1721:GLU:HB2	2.14	0.47
1:C:2453:ILE:HG12	1:C:2521:LEU:HD21	1.96	0.47
1:D:1010:ALA:O	1:D:1014:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1489:GLN:OE1	1:D:1489:GLN:N	2.45	0.47
1:B:320:VAL:HA	1:B:327:LEU:HA	1.97	0.47
1:C:95:MET:HB2	1:C:95:MET:HE2	1.71	0.47
1:C:1177:ALA:HB3	1:D:2176:PHE:HB2	1.97	0.47
1:D:408:GLU:O	1:D:412:GLY:HA3	2.15	0.47
1:D:1518:VAL:HG21	1:D:1553:ILE:HG12	1.96	0.47
1:D:1673:GLY:HA3	1:D:1731:LYS:HE2	1.97	0.47
1:B:961:LEU:HB2	1:B:966:ASP:HB3	1.96	0.47
1:B:2402:ASN:ND2	1:B:2419:ASP:OD2	2.48	0.47
1:C:357:PHE:HA	1:C:401:LEU:HG	1.97	0.47
1:C:902:LEU:O	1:C:903:ASN:HB2	2.14	0.47
1:D:1757:ASP:OD1	1:D:1757:ASP:N	2.47	0.47
1:E:1321:MET:HE3	1:E:1584:ILE:HG22	1.95	0.47
1:E:1483:VAL:HG13	1:E:1493:ILE:HG23	1.97	0.47
1:A:2311:LEU:HD22	1:A:2348:MET:HG2	1.96	0.47
1:D:414:LYS:HE3	1:D:414:LYS:HB3	1.78	0.47
1:D:687:ILE:HG23	1:D:745:LEU:HD21	1.97	0.47
1:D:2191:ALA:O	1:D:2195:VAL:HG13	2.14	0.47
1:E:1375:ILE:HA	1:E:1378:MET:HE2	1.97	0.47
1:E:2442:THR:HB	1:E:2529:ILE:HB	1.97	0.47
1:A:1631:VAL:HG11	1:B:1165:ARG:HB3	1.95	0.46
1:A:2515:THR:H	1:A:2516:ASP:CB	2.20	0.46
1:C:1116:ASN:HB2	1:D:1207:TRP:CD1	2.50	0.46
1:E:182:ASP:OD2	1:E:182:ASP:N	2.48	0.46
1:E:1418:THR:HG23	1:E:1419:LYS:HG3	1.97	0.46
1:E:1487:ASN:HB2	1:E:1492:GLN:HB3	1.97	0.46
1:A:127:LYS:HE2	1:A:127:LYS:HB3	1.63	0.46
1:A:1714:ALA:HB3	1:A:1717:TYR:HB2	1.97	0.46
1:A:2191:ALA:O	1:A:2195:VAL:HG13	2.16	0.46
1:B:95:MET:HE2	1:B:95:MET:HB2	1.74	0.46
1:B:300:LEU:HA	1:B:316:SER:O	2.15	0.46
1:C:1439:ILE:HD11	1:C:1486:ASN:HA	1.96	0.46
1:C:1570:VAL:HG22	1:C:1585:LYS:HG2	1.97	0.46
1:D:2350:LYS:HD2	1:E:2299:LEU:HD22	1.97	0.46
1:E:358:PHE:HB2	1:E:398:SER:HB3	1.96	0.46
1:A:1392:ALA:HB1	1:A:1417:LYS:NZ	2.31	0.46
1:C:304:TYR:HB3	1:C:308:THR:HG21	1.96	0.46
1:D:743:LEU:HD23	1:D:743:LEU:HA	1.82	0.46
1:A:26:GLN:N	1:A:27:TYR:HB3	2.30	0.46
1:A:1070:ARG:O	1:A:1074:GLU:HG3	2.15	0.46
1:A:1444:GLU:HB2	1:A:1481:TYR:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1531:ASP:OD1	1:C:1531:ASP:N	2.43	0.46
1:C:2101:ILE:HG12	1:D:2253:MET:HE3	1.96	0.46
1:D:14:THR:HB	1:D:20:MET:HE3	1.97	0.46
1:D:1610:ALA:HB2	1:D:1652:PRO:HG2	1.97	0.46
1:D:1738:TRP:HZ2	1:D:1770:VAL:HG11	1.80	0.46
1:A:6:VAL:O	1:A:10:LYS:HG3	2.14	0.46
1:A:618:TYR:OH	1:A:626:LYS:O	2.19	0.46
1:A:1451:LEU:HB2	1:A:1479:CYS:SG	2.56	0.46
1:A:1969:LEU:HD12	1:A:1969:LEU:H	1.80	0.46
1:A:2118:GLU:CD	1:A:2121:ARG:HH21	2.24	0.46
1:B:1409:GLY:HA3	1:B:1427:GLY:N	2.31	0.46
1:D:300:LEU:HA	1:D:316:SER:O	2.15	0.46
1:D:1738:TRP:CZ2	1:D:1770:VAL:HG11	2.50	0.46
1:D:2086:LEU:HD22	1:E:2271:LEU:HD13	1.97	0.46
1:B:200:HIS:HB3	1:B:203:TYR:HB3	1.98	0.46
1:B:2427:PRO:O	1:B:2434:ARG:NH2	2.46	0.46
1:C:1389:TYR:OH	1:C:1544:MET:HE1	2.15	0.46
1:D:360:ARG:NH1	1:D:362:ASN:HD21	2.13	0.46
1:D:554:THR:HG22	1:D:556:ALA:N	2.29	0.46
1:D:1907:ARG:NH1	1:E:158:GLU:OE1	2.46	0.46
1:B:1460:THR:O	1:B:1460:THR:HG23	2.14	0.46
1:C:1399:VAL:HG12	1:C:1497:TYR:HD2	1.80	0.46
1:C:2191:ALA:O	1:C:2195:VAL:HG13	2.16	0.46
1:C:2394:LYS:HB2	1:C:2394:LYS:HE2	1.76	0.46
1:E:414:LYS:HB3	1:E:414:LYS:HE3	1.77	0.46
1:E:1410:GLY:HA3	1:E:1497:TYR:CE1	2.51	0.46
1:A:300:LEU:HA	1:A:316:SER:O	2.15	0.46
1:A:902:LEU:O	1:A:903:ASN:HB2	2.15	0.46
1:A:1373:LYS:HD3	1:A:1412:ILE:HG13	1.97	0.46
1:A:2275:LYS:HD3	1:E:2079:ASP:HB3	1.98	0.46
1:D:2079:ASP:OD2	1:E:2277:THR:OG1	2.26	0.46
1:D:2134:TYR:CE1	1:D:2224:GLU:HB2	2.50	0.46
1:D:2277:THR:HA	1:D:2281:LEU:HD23	1.97	0.46
1:E:300:LEU:HA	1:E:316:SER:O	2.15	0.46
1:E:346:TYR:OH	1:E:395:ASN:OD1	2.26	0.46
1:B:360:ARG:HE	1:B:362:ASN:ND2	2.14	0.46
1:B:1758:ALA:O	1:B:1760:HIS:ND1	2.49	0.46
1:C:1575:ALA:HB2	1:C:1581:LEU:HD21	1.98	0.46
1:C:1760:HIS:HB2	1:C:1773:ILE:HB	1.98	0.46
1:D:350:MET:HE3	1:D:350:MET:HB3	1.88	0.46
1:D:1021:TRP:CE2	1:D:1025:ASN:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2515:THR:N	1:D:2516:ASP:HB2	2.18	0.46
1:A:1803:TRP:CZ2	1:A:1854:PRO:HB2	2.50	0.46
1:A:2264:HIS:NE2	1:E:2093:GLU:OE1	2.37	0.46
1:A:2394:LYS:HB2	1:A:2394:LYS:HE2	1.74	0.46
1:B:1174:GLU:OE2	1:B:1189:ARG:NH2	2.39	0.46
1:B:1760:HIS:HB2	1:B:1773:ILE:HB	1.98	0.46
1:C:1338:ILE:HG21	1:C:1354:LEU:HB3	1.98	0.46
1:C:1509:ILE:HG12	1:C:1514:ILE:HD11	1.98	0.46
1:D:91:SER:HB3	1:D:1960:LEU:HD11	1.98	0.46
1:E:369:PHE:HD2	1:E:387:SER:HA	1.81	0.46
1:E:561:MET:HG3	1:E:571:LEU:HD22	1.97	0.46
1:E:2394:LYS:HB2	1:E:2394:LYS:HE2	1.72	0.46
1:A:730:LEU:HD12	1:A:767:LEU:HD11	1.98	0.45
1:A:845:MET:HE2	1:A:845:MET:HB3	1.82	0.45
1:A:1148:THR:HG23	1:A:1150:VAL:HG23	1.98	0.45
1:A:1395:ILE:HG22	1:A:1414:VAL:HG22	1.96	0.45
1:B:299:MET:HE3	1:B:304:TYR:CD2	2.51	0.45
1:B:1430:MET:HE3	1:B:1430:MET:HB3	1.77	0.45
1:C:2219:ARG:O	1:C:2222:GLU:HG2	2.16	0.45
1:D:783:VAL:HG13	1:D:832:ARG:HG3	1.98	0.45
1:E:1108:TRP:CE2	1:E:1161:ILE:HD11	2.51	0.45
1:C:346:TYR:OH	1:C:395:ASN:OD1	2.25	0.45
1:C:829:ASP:OD1	1:C:832:ARG:NH2	2.47	0.45
1:D:2390:LEU:HD11	1:D:2522:LEU:HB2	1.97	0.45
1:E:409:TYR:CE1	1:E:414:LYS:HD3	2.51	0.45
1:E:1440:LEU:HB3	1:E:1479:CYS:HB3	1.98	0.45
1:A:415:ILE:HD13	1:A:434:PHE:HE2	1.81	0.45
1:A:2253:MET:HE1	1:E:2104:ARG:HG3	1.99	0.45
1:B:197:THR:O	1:B:453:ARG:NH1	2.48	0.45
1:B:1454:PHE:CZ	1:B:1468:VAL:HG22	2.51	0.45
1:C:345:ASN:ND2	1:C:362:ASN:O	2.49	0.45
1:D:1803:TRP:CZ2	1:D:1854:PRO:HB2	2.51	0.45
1:D:215:SER:O	1:D:216:THR:OG1	2.29	0.45
1:E:298:GLY:HA3	1:E:314:ASN:HB2	1.98	0.45
1:E:433:ILE:HD11	1:E:539:ALA:HB2	1.99	0.45
1:A:1365:GLY:H	1:A:1371:ARG:HD3	1.81	0.45
1:B:618:TYR:OH	1:B:626:LYS:O	2.24	0.45
1:B:2079:ASP:HB3	1:C:2275:LYS:HD3	1.98	0.45
1:C:505:VAL:HG11	1:C:598:TYR:HD2	1.80	0.45
1:C:1601:LEU:HD23	1:C:1615:LEU:HB2	1.99	0.45
1:D:1108:TRP:CE2	1:D:1161:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2439:VAL:HG22	1:D:2532:ILE:HG23	1.97	0.45
1:E:27:TYR:CD1	1:E:1947:GLN:HG3	2.52	0.45
1:E:1384:ASP:OD2	1:E:1385:GLY:N	2.47	0.45
1:E:1921:LEU:HD12	1:E:1921:LEU:HA	1.85	0.45
1:E:2219:ARG:HD3	1:E:2223:TRP:CZ2	2.52	0.45
1:B:347:PHE:CD1	1:B:415:ILE:HD11	2.52	0.45
1:B:507:ASN:OD1	1:B:507:ASN:C	2.60	0.45
1:C:2134:TYR:CE1	1:C:2224:GLU:HB2	2.51	0.45
1:D:247:TYR:CZ	1:D:898:TYR:HB3	2.52	0.45
1:D:1402:TYR:CE2	1:D:1481:TYR:HE1	2.35	0.45
1:A:566:VAL:HB	1:A:570:GLU:HB3	1.99	0.45
1:A:1308:ARG:O	1:A:1595:TYR:OH	2.34	0.45
1:A:1329:SER:O	1:A:1329:SER:OG	2.30	0.45
1:B:200:HIS:CE1	1:B:202:PRO:HG2	2.52	0.45
1:B:1485:GLY:HA3	1:B:1493:ILE:HA	1.99	0.45
1:C:899:VAL:O	1:C:900:THR:OG1	2.27	0.45
1:C:1308:ARG:O	1:C:1595:TYR:OH	2.32	0.45
1:C:1675:GLU:OE1	1:C:1677:TRP:NE1	2.37	0.45
1:D:415:ILE:HG12	1:D:431:GLY:CA	2.45	0.45
1:D:2079:ASP:HB3	1:E:2275:LYS:HD3	1.98	0.45
1:E:332:ILE:HG12	1:E:436:PHE:HD1	1.82	0.45
1:E:1724:ARG:HG2	1:E:1742:PHE:CZ	2.52	0.45
1:C:229:GLN:OE1	1:C:891:ARG:NH2	2.41	0.45
1:E:192:ARG:HG2	1:E:249:ILE:HD11	1.98	0.45
1:E:344:ILE:HA	1:E:361:ALA:O	2.17	0.45
1:A:197:THR:O	1:A:453:ARG:NH1	2.50	0.45
1:A:921:ASN:ND2	1:B:553:SER:OG	2.42	0.45
1:A:1108:TRP:CE2	1:A:1161:ILE:HD11	2.52	0.45
1:C:2129:LYS:NZ	1:D:2228:ASP:OD2	2.48	0.45
1:C:2488:PHE:HB2	1:D:2485:MET:HE3	1.98	0.45
1:D:226:VAL:HG12	1:D:876:TRP:CE2	2.52	0.45
1:A:358:PHE:HB2	1:A:398:SER:HB3	1.98	0.45
1:A:1927:GLU:OE2	1:A:1995:ARG:NH1	2.39	0.45
1:B:83:ILE:HD12	1:B:1880:MET:CE	2.47	0.45
1:B:743:LEU:HD13	1:B:757:LEU:HB2	1.99	0.45
1:B:1108:TRP:CE2	1:B:1161:ILE:HD11	2.52	0.45
1:C:1839:TYR:CE1	1:C:1851:ASN:HB2	2.52	0.45
1:C:2454:ARG:O	1:C:2512:PRO:HD2	2.16	0.45
1:C:2455:ALA:HB1	1:C:2509:LEU:HD11	1.99	0.45
1:D:1036:LEU:HD11	1:D:1871:PRO:HD3	1.98	0.45
1:D:2453:ILE:O	1:D:2475:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:HD13	1:E:11:ILE:HA	1.83	0.45
1:A:142:ARG:NH2	1:A:144:ASP:OD2	2.42	0.44
1:A:1443:VAL:HG13	1:A:1446:ASN:H	1.82	0.44
1:A:1633:ARG:NH2	1:A:1649:LEU:HD21	2.32	0.44
1:A:1673:GLY:HA3	1:A:1731:LYS:HE2	1.99	0.44
1:B:504:GLN:HG2	1:B:509:SER:HB2	1.99	0.44
1:C:1331:THR:HG21	1:C:1581:LEU:HD13	1.99	0.44
1:D:173:ILE:HD12	1:D:949:TRP:CE3	2.51	0.44
1:D:298:GLY:HA3	1:D:314:ASN:HB2	1.97	0.44
1:D:1426:GLN:HB3	1:D:1462:LEU:HB3	1.98	0.44
1:E:399:ASN:CG	1:E:399:ASN:O	2.59	0.44
1:E:531:PRO:HG3	1:E:535:LYS:HZ3	1.82	0.44
1:E:1010:ALA:O	1:E:1014:THR:HG23	2.17	0.44
1:E:1399:VAL:HG12	1:E:1497:TYR:HD2	1.83	0.44
1:E:2453:ILE:O	1:E:2475:SER:HA	2.17	0.44
1:B:344:ILE:HA	1:B:361:ALA:O	2.16	0.44
1:B:902:LEU:O	1:B:903:ASN:HB2	2.15	0.44
1:B:1415:TYR:HD1	1:B:1422:ILE:HD12	1.82	0.44
1:C:554:THR:HG22	1:C:556:ALA:N	2.28	0.44
1:D:1145:LYS:NZ	1:D:1147:ASP:OD1	2.50	0.44
1:E:2311:LEU:HD22	1:E:2348:MET:HG2	1.99	0.44
1:A:2161:VAL:HG23	1:D:1117:LEU:HD11	1.98	0.44
1:A:2390:LEU:HD12	1:A:2523:GLU:HG2	1.99	0.44
1:A:2453:ILE:O	1:A:2475:SER:HA	2.17	0.44
1:B:893:LEU:HD23	1:B:918:LEU:HD21	1.99	0.44
1:B:1365:GLY:H	1:B:1371:ARG:HD3	1.81	0.44
1:B:1381:THR:HB	1:B:1386:LYS:HA	1.99	0.44
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.60	0.44
1:C:1756:ASN:HB3	1:C:1773:ILE:HG23	1.99	0.44
1:D:1250:LYS:HD3	1:D:1296:THR:HG22	1.99	0.44
1:D:1724:ARG:HG2	1:D:1742:PHE:CZ	2.52	0.44
1:E:1757:ASP:OD1	1:E:1757:ASP:N	2.46	0.44
1:E:2191:ALA:O	1:E:2195:VAL:HG13	2.17	0.44
1:A:899:VAL:O	1:A:899:VAL:HG12	2.17	0.44
1:A:1399:VAL:HG12	1:A:1497:TYR:HD2	1.83	0.44
1:A:2388:GLN:O	1:A:2392:GLU:HG2	2.18	0.44
1:C:538:GLU:C	1:C:540:ASP:H	2.25	0.44
1:C:1724:ARG:HG2	1:C:1742:PHE:CZ	2.52	0.44
1:E:504:GLN:HG2	1:E:509:SER:HB2	1.99	0.44
1:E:1485:GLY:CA	1:E:1494:PHE:H	2.30	0.44
1:E:1677:TRP:CH2	1:E:1730:GLN:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HE3	1:A:350:MET:HB3	1.88	0.44
1:A:1150:VAL:HG11	1:A:1157:ILE:HD12	2.00	0.44
1:B:369:PHE:HD2	1:B:388:GLY:H	1.64	0.44
1:B:743:LEU:HD23	1:B:743:LEU:HA	1.81	0.44
1:B:1714:ALA:HB3	1:B:1717:TYR:HB2	2.00	0.44
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.74	0.44
1:D:473:ASN:ND2	1:D:477:ILE:H	2.15	0.44
1:D:1804:GLU:HA	1:D:1808:TYR:HB2	2.00	0.44
1:D:2282:TYR:O	1:D:2286:ARG:HG2	2.17	0.44
1:D:2364:ARG:NH2	1:D:2420:LEU:O	2.50	0.44
1:E:967:LEU:HD23	1:E:967:LEU:HA	1.84	0.44
1:E:2008:ASP:OD2	1:E:2010:GLN:HG2	2.16	0.44
1:A:297:LEU:O	1:A:316:SER:OG	2.26	0.44
1:A:1518:VAL:HG21	1:A:1553:ILE:HG12	1.98	0.44
1:A:2390:LEU:HD11	1:A:2522:LEU:HB3	2.00	0.44
1:C:115:PRO:HD2	1:C:155:MET:HE3	2.00	0.44
1:C:827:THR:HA	1:C:830:MET:HE2	1.99	0.44
1:C:1412:ILE:O	1:C:1424:SER:HA	2.18	0.44
1:D:337:THR:HA	1:D:537:PHE:CE2	2.53	0.44
1:E:783:VAL:HG13	1:E:832:ARG:HG3	1.99	0.44
1:A:1839:TYR:CE1	1:A:1851:ASN:HB2	2.53	0.44
1:B:27:TYR:HD2	1:B:28:LEU:HD22	1.83	0.44
1:B:288:LEU:HD21	1:B:456:LEU:HD21	2.00	0.44
1:C:103:PHE:CE2	1:C:1981:PRO:HB2	2.53	0.44
1:C:714:LEU:HD22	1:C:719:MET:HG2	1.99	0.44
1:C:921:ASN:ND2	1:D:553:SER:OG	2.47	0.44
1:C:2079:ASP:HB3	1:D:2275:LYS:HD3	1.99	0.44
1:C:2345:LEU:HA	1:C:2348:MET:HE3	1.99	0.44
1:D:321:VAL:HG12	1:D:326:LYS:O	2.18	0.44
1:D:505:VAL:HG11	1:D:598:TYR:HD2	1.83	0.44
1:D:1922:GLU:HB3	1:E:1004:ILE:HD13	1.99	0.44
1:D:2488:PHE:HB2	1:E:2485:MET:HE3	2.00	0.44
1:E:307:SER:C	1:E:309:SER:H	2.26	0.44
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.88	0.44
1:A:1426:GLN:HB3	1:A:1462:LEU:HD22	1.99	0.44
1:B:375:LYS:HA	1:B:375:LYS:HD3	1.70	0.44
1:B:2465:MET:HB3	1:B:2465:MET:HE3	1.80	0.44
1:C:621:SER:O	1:C:624:ASN:ND2	2.51	0.44
1:E:142:ARG:HD2	1:E:971:PHE:O	2.17	0.44
1:E:288:LEU:HD21	1:E:456:LEU:HD21	1.99	0.44
1:A:63:LEU:HD11	1:A:88:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.53	0.44
1:A:337:THR:HG23	1:A:432:GLY:HA2	1.99	0.44
1:A:360:ARG:CZ	1:A:362:ASN:HD21	2.31	0.44
1:A:538:GLU:CD	1:A:591:VAL:HG13	2.43	0.44
1:B:1333:MET:HE2	1:B:1359:PHE:CD1	2.52	0.44
1:B:1736:ASN:HB2	1:B:1739:GLU:CD	2.42	0.44
1:C:142:ARG:HD2	1:C:971:PHE:O	2.18	0.44
1:C:171:GLU:OE2	1:C:175:ARG:NH2	2.51	0.44
1:C:409:TYR:CE1	1:C:414:LYS:HD3	2.53	0.44
1:C:533:LYS:HD2	1:C:533:LYS:N	2.33	0.44
1:D:1674:ASP:HB2	1:D:1965:VAL:HG22	2.00	0.44
1:E:1374:GLN:NE2	1:E:1396:ALA:O	2.51	0.44
1:A:2453:ILE:HG23	1:A:2521:LEU:HD21	2.00	0.43
1:B:204:GLU:OE1	1:B:241:ASN:ND2	2.41	0.43
1:B:589:LEU:HD23	1:B:589:LEU:HA	1.86	0.43
1:B:1422:ILE:HG22	1:B:1466:PHE:HD2	1.83	0.43
1:B:1621:ARG:HB2	1:B:1654:LEU:HD21	1.99	0.43
1:D:2361:GLU:HG2	1:E:2484:PHE:CE2	2.53	0.43
1:E:419:ARG:HB3	1:E:429:GLN:HG3	1.99	0.43
1:A:505:VAL:HG11	1:A:598:TYR:CD2	2.53	0.43
1:A:1394:ILE:HB	1:A:1415:TYR:HB3	2.00	0.43
1:A:2049:ARG:HG3	1:A:2491:SER:O	2.18	0.43
1:B:1485:GLY:HA3	1:B:1494:PHE:H	1.84	0.43
1:B:2106:VAL:O	1:B:2109:VAL:HG22	2.18	0.43
1:D:373:LEU:HB2	1:D:416:TYR:CB	2.47	0.43
1:E:730:LEU:HD12	1:E:767:LEU:HD11	1.99	0.43
1:E:2514:ALA:HB1	1:E:2522:LEU:HD22	1.99	0.43
1:A:2442:THR:HB	1:A:2529:ILE:HB	2.01	0.43
1:B:1438:LEU:O	1:B:1453:GLU:HA	2.18	0.43
1:B:1757:ASP:OD1	1:B:1757:ASP:N	2.46	0.43
1:C:620:LEU:HD22	1:C:664:CYS:HB3	2.01	0.43
1:C:1373:LYS:HG3	1:C:1412:ILE:HG13	1.99	0.43
1:C:2092:MET:HG2	1:C:2265:THR:HG22	2.00	0.43
1:D:344:ILE:HA	1:D:361:ALA:O	2.18	0.43
1:E:197:THR:O	1:E:453:ARG:NH1	2.52	0.43
1:E:270:ASN:O	1:E:1445:ASN:ND2	2.52	0.43
1:E:1368:ASN:ND2	1:E:1370:ILE:HB	2.33	0.43
1:E:2364:ARG:NH2	1:E:2420:LEU:O	2.52	0.43
1:A:1036:LEU:HD11	1:A:1871:PRO:HD3	2.01	0.43
1:B:1824:ASP:OD1	1:B:1897:ARG:NH2	2.51	0.43
1:C:1035:ARG:NH2	1:C:1982:GLU:OE2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:VAL:HB	1:C:1593:VAL:HG22	1.99	0.43
1:C:2106:VAL:O	1:C:2109:VAL:HG22	2.19	0.43
1:D:1365:GLY:H	1:D:1371:ARG:HD3	1.83	0.43
1:E:1457:SER:HB3	1:E:1458:PRO:CD	2.46	0.43
1:B:317:THR:HG22	1:B:330:TYR:CE2	2.54	0.43
1:B:2364:ARG:NH2	1:B:2420:LEU:O	2.51	0.43
1:D:247:TYR:OH	1:D:900:THR:N	2.51	0.43
1:D:1844:GLU:HG3	1:D:1845:ILE:N	2.34	0.43
1:E:320:VAL:HA	1:E:327:LEU:HA	2.00	0.43
1:A:95:MET:HE2	1:A:95:MET:HB2	1.83	0.43
1:A:136:TYR:CZ	1:A:959:VAL:HG22	2.53	0.43
1:C:2026:LEU:HD12	1:C:2026:LEU:HA	1.88	0.43
1:D:76:SER:N	1:D:77:GLY:HA3	2.34	0.43
1:D:420:TYR:CD2	1:D:426:ALA:HB2	2.54	0.43
1:D:810:LEU:HD12	1:D:810:LEU:HA	1.84	0.43
1:E:1677:TRP:CZ2	1:E:1730:GLN:HB2	2.53	0.43
1:B:142:ARG:HD2	1:B:971:PHE:O	2.18	0.43
1:B:620:LEU:HB3	1:B:804:ILE:HG13	2.01	0.43
1:B:1631:VAL:HG11	1:C:1165:ARG:HB3	2.01	0.43
1:B:1744:TYR:CE1	1:B:1753:VAL:HB	2.53	0.43
1:C:365:VAL:HG22	1:C:391:ILE:HA	2.00	0.43
1:C:680:LEU:HD22	1:C:744:VAL:HG22	1.99	0.43
1:C:1412:ILE:HB	1:C:1425:VAL:HG12	2.00	0.43
1:D:1839:TYR:CE1	1:D:1851:ASN:HB2	2.53	0.43
1:D:1907:ARG:HH22	1:E:158:GLU:CD	2.26	0.43
1:A:350:MET:HG3	1:A:359:ILE:HG13	2.01	0.43
1:A:687:ILE:HD11	1:A:741:MET:HG2	1.99	0.43
1:B:680:LEU:HD11	1:B:757:LEU:HD21	2.00	0.43
1:B:1100:VAL:HB	1:B:1593:VAL:HG22	2.00	0.43
1:B:1169:ILE:HD11	1:B:1192:LEU:HD11	2.01	0.43
1:B:1969:LEU:HD12	1:B:1969:LEU:H	1.84	0.43
1:C:415:ILE:HG12	1:C:431:GLY:CA	2.41	0.43
1:C:473:ASN:ND2	1:C:477:ILE:H	2.17	0.43
1:C:1764:MET:HE1	1:C:1768:GLY:HA2	2.01	0.43
1:C:1922:GLU:HB3	1:D:1004:ILE:HD13	2.01	0.43
1:D:1744:TYR:CE1	1:D:1753:VAL:HB	2.54	0.43
1:E:242:ILE:HA	1:E:246:LEU:HD23	2.01	0.43
1:E:247:TYR:OH	1:E:900:THR:N	2.51	0.43
1:E:676:ILE:O	1:E:680:LEU:HG	2.19	0.43
1:E:680:LEU:HD22	1:E:744:VAL:HG22	2.01	0.43
1:E:1480:SER:OG	1:E:1481:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:LYS:HB3	1:A:1528:THR:HG22	2.01	0.43
1:B:321:VAL:HG12	1:B:326:LYS:O	2.19	0.43
1:B:2394:LYS:HE2	1:B:2394:LYS:HB2	1.78	0.43
1:C:2350:LYS:HD2	1:D:2299:LEU:HD22	2.00	0.43
1:E:500:PHE:HD1	1:E:500:PHE:HA	1.72	0.43
1:A:570:GLU:HG2	1:A:611:VAL:HB	2.01	0.43
1:A:1744:TYR:CE1	1:A:1753:VAL:HB	2.54	0.43
1:A:2176:PHE:HB2	1:E:1177:ALA:HB3	2.00	0.43
1:A:2282:TYR:O	1:A:2286:ARG:HG2	2.19	0.43
1:B:82:GLY:C	1:B:83:ILE:HD13	2.44	0.43
1:B:1302:VAL:HG23	1:B:1604:ARG:HG2	2.00	0.43
1:C:2514:ALA:HB1	1:C:2522:LEU:HD22	2.00	0.43
1:C:2519:LYS:NZ	1:C:2523:GLU:OE1	2.46	0.43
1:E:554:THR:HG22	1:E:556:ALA:N	2.31	0.43
1:A:238:ILE:HD13	1:A:238:ILE:HA	1.94	0.42
1:A:294:GLN:OE1	1:E:1934:GLN:NE2	2.43	0.42
1:A:414:LYS:HE3	1:A:414:LYS:HB3	1.88	0.42
1:A:912:TRP:NE1	1:A:916:GLN:HE21	2.17	0.42
1:A:1218:VAL:HG21	1:A:1245:VAL:HG12	2.01	0.42
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.87	0.42
1:C:2442:THR:HB	1:C:2529:ILE:HB	2.00	0.42
1:D:473:ASN:ND2	1:D:477:ILE:HG12	2.33	0.42
1:D:730:LEU:HD12	1:D:767:LEU:HD11	2.00	0.42
1:E:1437:ARG:HG2	1:E:1486:ASN:CB	2.48	0.42
1:A:1757:ASP:OD1	1:A:1757:ASP:N	2.44	0.42
1:A:2219:ARG:HD3	1:A:2223:TRP:CZ2	2.54	0.42
1:A:2219:ARG:O	1:A:2222:GLU:HG2	2.19	0.42
1:B:242:ILE:HA	1:B:246:LEU:HD23	2.01	0.42
1:B:305:SER:OG	1:B:306:ASP:N	2.52	0.42
1:B:419:ARG:HB3	1:B:429:GLN:HG3	2.02	0.42
1:B:1372:ASN:C	1:B:1373:LYS:HD3	2.43	0.42
1:B:1452:PHE:HZ	1:B:1472:LYS:HB3	1.84	0.42
1:C:373:LEU:C	1:C:416:TYR:HB2	2.44	0.42
1:A:581:LEU:HD23	1:A:581:LEU:HA	1.86	0.42
1:A:1456:PHE:HB3	1:A:1458:PRO:O	2.19	0.42
1:A:2074:MET:HE1	1:A:2285:MET:HB3	2.01	0.42
1:A:2361:GLU:HG2	1:B:2484:PHE:CE2	2.54	0.42
1:B:14:THR:HB	1:B:20:MET:HB2	2.00	0.42
1:B:1148:THR:HG23	1:B:1150:VAL:HG23	2.01	0.42
1:B:1518:VAL:HG21	1:B:1553:ILE:HG12	2.01	0.42
1:C:199:TYR:CD1	1:C:945:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:LEU:HD21	1:C:704:LEU:HD22	2.01	0.42
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.53	0.42
1:D:247:TYR:OH	1:D:480:ASP:OD1	2.25	0.42
1:D:561:MET:HG3	1:D:571:LEU:HD22	2.01	0.42
1:D:1457:SER:HB2	1:D:1458:PRO:HD3	2.00	0.42
1:E:415:ILE:HG12	1:E:431:GLY:CA	2.48	0.42
1:E:2385:LYS:HE3	1:E:2397:VAL:HG21	2.00	0.42
1:A:1:MET:HB2	1:A:1564:ILE:HG23	2.01	0.42
1:A:1207:TRP:CD1	1:E:1116:ASN:HB2	2.54	0.42
1:A:1368:ASN:N	1:A:1368:ASN:OD1	2.51	0.42
1:A:1555:ALA:HB1	1:A:1558:LEU:HD11	2.01	0.42
1:A:2106:VAL:O	1:A:2109:VAL:HG22	2.18	0.42
1:B:1456:PHE:HB3	1:B:1458:PRO:O	2.19	0.42
1:C:347:PHE:HE2	1:C:417:ALA:HB2	1.85	0.42
1:C:922:MET:HE3	1:C:922:MET:HB3	1.87	0.42
1:C:2361:GLU:HG2	1:D:2484:PHE:CE2	2.55	0.42
1:D:1570:VAL:HG22	1:D:1585:LYS:HG2	2.01	0.42
1:E:91:SER:HB3	1:E:1960:LEU:HD11	2.01	0.42
1:E:1536:LEU:HD13	1:E:1537:PRO:HD2	2.01	0.42
1:A:854:GLN:OE1	1:A:886:MET:HE3	2.19	0.42
1:A:2228:ASP:OD2	1:E:2129:LYS:NZ	2.52	0.42
1:B:675:GLU:HG3	1:B:676:ILE:N	2.35	0.42
1:B:1478:LYS:N	1:B:1478:LYS:HD3	2.34	0.42
1:C:197:THR:O	1:C:453:ARG:NH1	2.53	0.42
1:C:271:ILE:HD13	1:C:281:TRP:HZ2	1.85	0.42
1:C:546:ILE:HD11	1:C:581:LEU:HD21	2.01	0.42
1:C:783:VAL:HG13	1:C:832:ARG:HG3	2.01	0.42
1:C:1630:LEU:HD22	1:C:1641:ILE:HG23	2.02	0.42
1:C:1795:ASN:O	1:C:1795:ASN:ND2	2.48	0.42
1:C:2426:TYR:HB2	1:C:2434:ARG:HH12	1.85	0.42
1:D:309:SER:OG	1:D:310:ALA:N	2.53	0.42
1:D:2057:THR:HG22	1:D:2345:LEU:HD11	2.02	0.42
1:D:2192:SER:O	1:D:2195:VAL:HG22	2.19	0.42
1:E:299:MET:HE3	1:E:304:TYR:CD2	2.55	0.42
1:E:365:VAL:HG22	1:E:391:ILE:HA	2.01	0.42
1:E:856:MET:HB3	1:E:856:MET:HE3	1.75	0.42
1:E:1380:LEU:HD21	1:E:1463:ASN:HB3	2.01	0.42
1:A:415:ILE:HG12	1:A:431:GLY:CA	2.49	0.42
1:B:1436:ARG:HG2	1:B:1456:PHE:CD2	2.55	0.42
1:B:2070:SER:O	1:B:2074:MET:HG3	2.20	0.42
1:B:2359:ALA:HB2	1:B:2537:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1803:TRP:CZ2	1:C:1854:PRO:HB2	2.54	0.42
1:D:1401:HIS:HB2	1:D:1497:TYR:CZ	2.55	0.42
1:E:360:ARG:HE	1:E:362:ASN:ND2	2.18	0.42
1:E:1333:MET:HE3	1:E:1333:MET:HB2	1.91	0.42
1:A:20:MET:HE2	1:A:20:MET:HB2	1.91	0.42
1:A:347:PHE:HE2	1:A:417:ALA:HB2	1.83	0.42
1:A:680:LEU:HD22	1:A:744:VAL:HG22	2.00	0.42
1:A:1443:VAL:CG1	1:A:1446:ASN:H	2.32	0.42
1:A:2192:SER:O	1:A:2195:VAL:HG22	2.20	0.42
1:A:2192:SER:O	1:A:2196:MET:HG2	2.19	0.42
1:B:2057:THR:HG22	1:B:2345:LEU:HD11	2.00	0.42
1:C:95:MET:HE1	1:C:1959:MET:HE1	2.02	0.42
1:C:200:HIS:CE1	1:C:202:PRO:HG2	2.54	0.42
1:C:1437:ARG:HB3	1:C:1455:PRO:HA	2.01	0.42
1:C:1907:ARG:NH1	1:D:158:GLU:OE1	2.50	0.42
1:C:2465:MET:HE3	1:C:2465:MET:HB3	1.86	0.42
1:C:2526:SER:OG	1:C:2527:ASP:N	2.53	0.42
1:D:374:ARG:HE	1:D:374:ARG:HB3	1.64	0.42
1:D:1624:THR:HG1	1:D:1802:TYR:HH	1.36	0.42
1:D:1639:ASP:O	1:D:1643:THR:HG23	2.20	0.42
1:E:556:ALA:HB1	1:E:589:LEU:HD11	2.01	0.42
1:A:2136:GLU:OE2	1:B:2218:ARG:NH1	2.51	0.42
1:B:173:ILE:HD12	1:B:949:TRP:CE3	2.55	0.42
1:B:226:VAL:HG12	1:B:876:TRP:CE2	2.54	0.42
1:B:271:ILE:HD13	1:B:281:TRP:HZ2	1.85	0.42
1:B:1410:GLY:HA3	1:B:1497:TYR:CE1	2.54	0.42
1:C:1344:LYS:HB3	1:C:1344:LYS:HE3	1.81	0.42
1:D:231:GLU:HG3	1:D:897:ARG:HB3	2.02	0.42
1:D:372:THR:HA	1:D:416:TYR:O	2.20	0.42
1:D:436:PHE:CZ	1:D:438:SER:HB2	2.54	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.73	0.42
1:A:181:SER:O	1:A:185:MET:HG2	2.20	0.42
1:A:2057:THR:HG22	1:A:2345:LEU:HD11	2.02	0.42
1:B:247:TYR:OH	1:B:480:ASP:OD1	2.23	0.42
1:B:420:TYR:CD1	1:B:426:ALA:HB2	2.55	0.42
1:B:1825:GLU:OE1	1:B:1825:GLU:N	2.45	0.42
1:B:2488:PHE:HD2	1:C:2485:MET:HE3	1.84	0.42
1:C:1510:ASN:HB2	1:C:1513:ASP:HB2	2.01	0.42
1:D:142:ARG:HD2	1:D:971:PHE:O	2.20	0.42
1:D:1731:LYS:HD3	1:D:1731:LYS:N	2.35	0.42
1:E:83:ILE:HG23	1:E:1880:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2364:ARG:HB3	1:E:2532:ILE:HG13	2.02	0.42
1:A:76:SER:N	1:A:77:GLY:HA3	2.35	0.42
1:A:1228:LEU:HD11	1:A:1245:VAL:HG13	2.02	0.42
1:A:1922:GLU:HB3	1:B:1004:ILE:HD13	2.01	0.42
1:A:2137:ASP:O	1:B:2218:ARG:NH2	2.53	0.42
1:B:642:TRP:CZ2	1:B:646:VAL:HG21	2.55	0.42
1:B:902:LEU:HD23	1:B:902:LEU:HA	1.92	0.42
1:B:1400:LYS:HG2	1:B:1498:GLN:HB2	2.01	0.42
1:C:406:ASP:HA	1:C:409:TYR:HD2	1.84	0.42
1:C:1368:ASN:OD1	1:C:1368:ASN:N	2.53	0.42
1:C:1374:GLN:HE22	1:C:1396:ALA:H	1.67	0.42
1:C:1419:LYS:HB3	1:C:1421:TYR:CE1	2.55	0.42
1:C:1468:VAL:HG12	1:C:1470:SER:H	1.84	0.42
1:C:2368:LEU:HD23	1:C:2368:LEU:HA	1.84	0.42
1:D:367:ARG:HA	1:D:367:ARG:HD3	1.88	0.42
1:E:1315:VAL:HG11	1:E:1343:SER:HB2	2.00	0.42
1:E:1731:LYS:HD3	1:E:1731:LYS:N	2.35	0.42
1:A:173:ILE:HD12	1:A:949:TRP:CE3	2.54	0.41
1:A:1123:ARG:HD2	1:A:1143:TRP:CE2	2.55	0.41
1:A:1575:ALA:HB2	1:A:1581:LEU:HD21	2.01	0.41
1:A:2376:SER:OG	1:A:2377:SER:N	2.53	0.41
1:B:414:LYS:HE3	1:B:414:LYS:HB3	1.81	0.41
1:B:683:LEU:HD21	1:B:704:LEU:HD22	2.02	0.41
1:B:687:ILE:HG23	1:B:745:LEU:HD21	2.02	0.41
1:B:1960:LEU:HD12	1:B:1960:LEU:HA	1.87	0.41
1:B:2434:ARG:HG2	1:B:2536:ILE:HG23	2.02	0.41
1:C:288:LEU:HD21	1:C:456:LEU:HD21	2.01	0.41
1:C:414:LYS:HB3	1:C:414:LYS:HE3	1.74	0.41
1:C:1388:GLN:HG3	1:C:1416:ASN:ND2	2.35	0.41
1:D:345:ASN:HB2	1:D:361:ALA:HB3	2.02	0.41
1:D:1824:ASP:OD1	1:D:1897:ARG:NH2	2.53	0.41
1:E:162:LEU:HD23	1:E:162:LEU:HA	1.77	0.41
1:E:1146:ILE:HG22	1:E:1148:THR:HG22	2.02	0.41
1:E:1399:VAL:HG13	1:E:1498:GLN:O	2.20	0.41
1:B:247:TYR:OH	1:B:900:THR:N	2.52	0.41
1:B:1380:LEU:HD21	1:B:1463:ASN:HB3	2.02	0.41
1:B:2371:PHE:CE2	1:B:2415:VAL:HG13	2.55	0.41
1:C:298:GLY:HA3	1:C:314:ASN:HB2	2.01	0.41
1:C:415:ILE:HG13	1:C:416:TYR:N	2.34	0.41
1:D:1135:LEU:HD12	1:D:1135:LEU:HA	1.91	0.41
1:D:1371:ARG:NH1	1:D:1375:ILE:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2339:GLU:HG3	1:E:2067:PHE:CE1	2.55	0.41
1:E:127:LYS:HB3	1:E:127:LYS:HE2	1.69	0.41
1:E:566:VAL:HB	1:E:570:GLU:HB2	2.02	0.41
1:A:433:ILE:HD11	1:A:539:ALA:HB2	2.03	0.41
1:A:1425:VAL:HG13	1:A:1463:ASN:OD1	2.19	0.41
1:B:783:VAL:HG13	1:B:832:ARG:HG3	2.03	0.41
1:B:2417:LEU:HD23	1:B:2417:LEU:HA	1.93	0.41
1:C:501:ASP:HB3	1:C:522:HIS:ND1	2.35	0.41
1:A:554:THR:HG22	1:A:556:ALA:N	2.34	0.41
1:A:1731:LYS:N	1:A:1731:LYS:HD3	2.35	0.41
1:A:1907:ARG:HH12	1:B:158:GLU:CD	2.28	0.41
1:A:2465:MET:HE3	1:A:2465:MET:HB3	1.83	0.41
1:B:365:VAL:HG22	1:B:391:ILE:HA	2.02	0.41
1:B:1650:PRO:HA	1:B:1791:PRO:HA	2.02	0.41
1:C:507:ASN:OD1	1:C:507:ASN:C	2.63	0.41
1:C:1610:ALA:HB2	1:C:1652:PRO:HG2	2.01	0.41
1:C:1763:GLY:O	1:C:1769:ILE:HA	2.20	0.41
1:D:473:ASN:OD1	1:D:473:ASN:N	2.54	0.41
1:E:208:GLN:HG3	1:E:937:TYR:CD2	2.55	0.41
1:E:784:LEU:HD13	1:E:810:LEU:HD11	2.01	0.41
1:E:2214:GLU:O	1:E:2218:ARG:HG2	2.20	0.41
1:A:305:SER:OG	1:A:306:ASP:N	2.54	0.41
1:A:307:SER:C	1:A:309:SER:H	2.28	0.41
1:B:309:SER:OG	1:B:310:ALA:N	2.53	0.41
1:B:902:LEU:C	1:B:904:LYS:H	2.28	0.41
1:B:1689:THR:OG1	1:B:1719:MET:HE1	2.19	0.41
1:C:419:ARG:HB3	1:C:429:GLN:HG3	2.02	0.41
1:C:792:LEU:HD22	1:C:810:LEU:HD13	2.03	0.41
1:C:1759:ASP:OD1	1:C:1774:LYS:HA	2.20	0.41
1:D:242:ILE:HA	1:D:246:LEU:HD23	2.02	0.41
1:D:784:LEU:HD13	1:D:810:LEU:HD11	2.01	0.41
1:D:1742:PHE:O	1:D:1754:LEU:HD12	2.20	0.41
1:D:2426:TYR:HB2	1:D:2434:ARG:HH12	1.85	0.41
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.81	0.41
1:E:642:TRP:CZ2	1:E:646:VAL:HG21	2.55	0.41
1:E:2026:LEU:HD12	1:E:2026:LEU:HA	1.86	0.41
1:E:2519:LYS:O	1:E:2523:GLU:HG3	2.20	0.41
1:A:899:VAL:O	1:A:899:VAL:CG1	2.69	0.41
1:A:1410:GLY:HA3	1:A:1497:TYR:CE1	2.56	0.41
1:A:2094:LEU:HD23	1:A:2094:LEU:HA	1.91	0.41
1:C:1451:LEU:HB2	1:C:1479:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:HD22	1:D:45:GLU:HB3	2.03	0.41
1:D:1969:LEU:HD12	1:D:1969:LEU:H	1.86	0.41
1:E:247:TYR:OH	1:E:480:ASP:OD1	2.23	0.41
1:E:1148:THR:HG23	1:E:1150:VAL:HG23	2.02	0.41
1:E:2526:SER:OG	1:E:2527:ASP:N	2.54	0.41
1:A:192:ARG:NH1	1:A:245:GLU:OE2	2.51	0.41
1:A:1921:LEU:HD12	1:A:1921:LEU:HA	1.92	0.41
1:A:2273:GLN:HG2	1:E:2030:MET:HE3	2.01	0.41
1:B:845:MET:HE2	1:B:845:MET:HB3	1.80	0.41
1:B:886:MET:CE	1:C:569:GLY:H	2.32	0.41
1:B:1398:THR:O	1:B:1500:SER:OG	2.38	0.41
1:B:1731:LYS:HD3	1:B:1731:LYS:N	2.36	0.41
1:B:1742:PHE:O	1:B:1754:LEU:HD12	2.20	0.41
1:B:2092:MET:SD	1:B:2265:THR:HG22	2.60	0.41
1:C:1441:THR:O	1:C:1481:TYR:HB2	2.21	0.41
1:D:2368:LEU:HD23	1:D:2368:LEU:HA	1.74	0.41
1:D:2434:ARG:HG2	1:D:2536:ILE:HG23	2.02	0.41
1:D:2526:SER:OG	1:D:2527:ASP:N	2.53	0.41
1:E:304:TYR:HB3	1:E:308:THR:HG21	2.03	0.41
1:E:728:ASP:HB2	1:E:737:ILE:HG13	2.03	0.41
1:E:839:ASP:HA	1:E:849:ILE:HD13	2.02	0.41
1:E:902:LEU:C	1:E:904:LYS:H	2.28	0.41
1:E:1839:TYR:CE1	1:E:1851:ASN:HB2	2.56	0.41
1:A:466:GLN:O	1:A:470:ARG:HG3	2.20	0.41
1:A:504:GLN:HA	1:A:507:ASN:HD21	1.86	0.41
1:B:27:TYR:CD1	1:B:1947:GLN:HG3	2.55	0.41
1:B:538:GLU:C	1:B:540:ASP:H	2.28	0.41
1:B:1365:GLY:HA3	1:B:1371:ARG:HB2	2.01	0.41
1:C:26:GLN:NE2	1:C:57:LYS:HG3	2.36	0.41
1:C:505:VAL:HG11	1:C:598:TYR:CD2	2.55	0.41
1:C:1021:TRP:CE2	1:C:1025:ASN:HB3	2.56	0.41
1:D:2332:THR:HA	1:E:2281:LEU:HD12	2.03	0.41
1:E:173:ILE:HD12	1:E:949:TRP:CE3	2.56	0.41
1:E:1430:MET:HE3	1:E:1430:MET:HB3	1.99	0.41
1:E:1633:ARG:NH2	1:E:1649:LEU:HD21	2.34	0.41
1:A:460:LEU:HD23	1:A:500:PHE:HD1	1.86	0.41
1:A:1630:LEU:HD22	1:A:1641:ILE:HG23	2.02	0.41
1:B:41:LEU:HD22	1:B:45:GLU:HB3	2.03	0.41
1:B:208:GLN:HG3	1:B:937:TYR:CD2	2.56	0.41
1:B:297:LEU:O	1:B:316:SER:OG	2.31	0.41
1:B:403:ASN:O	1:B:404:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:PRO:HG2	1:B:443:ILE:HD12	2.02	0.41
1:B:1117:LEU:HD12	1:B:1117:LEU:HA	1.95	0.41
1:B:1274:LYS:HE3	1:B:1274:LYS:HB2	1.92	0.41
1:B:1392:ALA:HB3	1:B:1417:LYS:HG2	2.03	0.41
1:B:1923:LEU:HD23	1:B:1923:LEU:HA	1.94	0.41
1:B:2192:SER:O	1:B:2195:VAL:HG22	2.21	0.41
1:C:82:GLY:C	1:C:83:ILE:HD13	2.46	0.41
1:C:242:ILE:HA	1:C:246:LEU:HD23	2.03	0.41
1:C:1365:GLY:HA3	1:C:1371:ARG:HB2	2.03	0.41
1:C:2282:TYR:O	1:C:2286:ARG:HG2	2.20	0.41
1:C:2519:LYS:HZ1	1:C:2523:GLU:CD	2.27	0.41
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.93	0.41
1:D:347:PHE:CD2	1:D:415:ILE:HD11	2.56	0.41
1:D:369:PHE:CD2	1:D:387:SER:HA	2.56	0.41
1:D:538:GLU:H	1:D:538:GLU:HG3	1.58	0.41
1:D:1624:THR:OG1	1:D:1802:TYR:OH	2.14	0.41
1:D:1667:TYR:OH	1:D:1673:GLY:O	2.24	0.41
1:E:50:TYR:O	1:E:54:ILE:HG12	2.21	0.41
1:E:498:LEU:HD11	1:E:606:VAL:HG11	2.03	0.41
1:E:535:LYS:HA	1:E:535:LYS:HD3	1.96	0.41
1:E:751:ALA:C	1:E:753:GLU:H	2.29	0.41
1:E:2313:ARG:HH22	1:E:2465:MET:HE2	1.86	0.41
1:C:1456:PHE:HB3	1:C:1458:PRO:O	2.21	0.41
1:C:1485:GLY:HA2	1:C:1494:PHE:CD1	2.56	0.41
1:D:1452:PHE:CZ	1:D:1472:LYS:HD3	2.55	0.41
1:A:304:TYR:HB3	1:A:308:THR:HG21	2.03	0.40
1:A:347:PHE:CE1	1:A:415:ILE:HD11	2.55	0.40
1:A:902:LEU:C	1:A:904:LYS:H	2.28	0.40
1:A:1412:ILE:HB	1:A:1425:VAL:HB	2.02	0.40
1:A:2526:SER:OG	1:A:2527:ASP:N	2.53	0.40
1:B:415:ILE:HD13	1:B:434:PHE:HE2	1.86	0.40
1:B:1927:GLU:HB2	1:B:1991:TRP:CD2	2.56	0.40
1:C:91:SER:HB3	1:C:1960:LEU:HD11	2.03	0.40
1:C:1221:LYS:HE2	1:C:1221:LYS:HB2	1.87	0.40
1:C:1300:ASP:OD2	1:C:1604:ARG:NH2	2.42	0.40
1:D:1277:GLU:O	1:D:1281:LEU:HB2	2.21	0.40
1:D:1677:TRP:HA	1:D:1698:MET:HA	2.04	0.40
1:E:239:LEU:HD23	1:E:239:LEU:HA	1.91	0.40
1:E:1130:MET:HG3	1:E:1135:LEU:HD13	2.03	0.40
1:E:1969:LEU:H	1:E:1969:LEU:HD12	1.84	0.40
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2368:LEU:HD21	1:A:2415:VAL:HG21	2.03	0.40
1:B:141:ARG:NH2	1:B:1005:GLU:OE2	2.41	0.40
1:B:365:VAL:HG22	1:B:392:ALA:H	1.85	0.40
1:B:1011:ASP:OD1	1:B:1011:ASP:N	2.47	0.40
1:B:1040:PRO:O	1:B:1044:ILE:HG12	2.21	0.40
1:B:1959:MET:HB3	1:B:1959:MET:HE2	1.89	0.40
1:B:2026:LEU:HD12	1:B:2026:LEU:HA	1.94	0.40
1:B:2161:VAL:HG23	1:E:1117:LEU:HD11	2.02	0.40
1:C:784:LEU:HD13	1:C:810:LEU:HD11	2.03	0.40
1:C:1458:PRO:HD2	1:C:1461:ILE:HG21	2.02	0.40
1:D:618:TYR:OH	1:D:626:LYS:O	2.21	0.40
1:D:728:ASP:O	1:D:731:ARG:HG2	2.21	0.40
1:D:752:ASN:OD1	1:D:752:ASN:C	2.64	0.40
1:E:14:THR:HG22	1:E:18:GLN:O	2.21	0.40
1:E:504:GLN:O	1:E:507:ASN:ND2	2.53	0.40
1:E:505:VAL:HG11	1:E:598:TYR:HD2	1.87	0.40
1:A:1399:VAL:HG13	1:A:1498:GLN:O	2.22	0.40
1:A:2514:ALA:HB1	1:A:2522:LEU:HD22	2.02	0.40
1:B:460:LEU:HD23	1:B:460:LEU:HA	1.90	0.40
1:B:1839:TYR:CE1	1:B:1851:ASN:HB2	2.56	0.40
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.92	0.40
1:D:1633:ARG:NH2	1:D:1649:LEU:HD21	2.36	0.40
1:D:2349:GLU:OE2	1:E:2056:ARG:NH1	2.51	0.40
1:E:1730:GLN:O	1:E:1731:LYS:HB2	2.22	0.40
1:A:233:ALA:HB3	1:A:898:TYR:HB2	2.04	0.40
1:A:397:LYS:HB3	1:A:397:LYS:HE3	1.89	0.40
1:A:1985:PRO:HA	1:A:1988:THR:OG1	2.22	0.40
1:B:501:ASP:HB3	1:B:522:HIS:ND1	2.36	0.40
1:B:1451:LEU:HB2	1:B:1479:CYS:SG	2.61	0.40
1:B:2453:ILE:O	1:B:2475:SER:HA	2.20	0.40
1:D:703:ILE:HD13	1:D:703:ILE:HA	1.95	0.40
1:D:2348:MET:O	1:D:2351:VAL:HG12	2.22	0.40
1:D:2454:ARG:O	1:D:2512:PRO:HD2	2.22	0.40
1:D:2459:TYR:CZ	1:D:2461:GLY:HA3	2.56	0.40
1:E:282:ILE:HD12	1:E:297:LEU:HD11	2.03	0.40
1:E:420:TYR:CD1	1:E:426:ALA:HB2	2.57	0.40
1:A:11:ILE:HG22	1:A:20:MET:HE3	2.04	0.40
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.91	0.40
1:A:1409:GLY:HA3	1:A:1427:GLY:N	2.37	0.40
1:A:2368:LEU:HD23	1:A:2368:LEU:HA	1.77	0.40
1:B:1321:MET:HB3	1:B:1584:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:O	1:C:53:THR:HG21	2.22	0.40
1:C:1410:GLY:HA3	1:C:1497:TYR:CE1	2.57	0.40
1:D:902:LEU:C	1:D:904:LYS:H	2.27	0.40
1:D:1376:SER:HA	1:D:1379:LYS:HB2	2.04	0.40
1:E:1430:MET:HG3	1:E:1494:PHE:CD1	2.52	0.40
1:E:1714:ALA:HB3	1:E:1717:TYR:HB2	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%)	2415 (95%)	112 (4%)	8 (0%)	36	67
1	B	2535/2538 (100%)	2420 (96%)	107 (4%)	8 (0%)	36	67
1	C	2535/2538 (100%)	2417 (95%)	111 (4%)	7 (0%)	36	67
1	D	2535/2538 (100%)	2426 (96%)	101 (4%)	8 (0%)	36	67
1	E	2535/2538 (100%)	2417 (95%)	110 (4%)	8 (0%)	36	67
All	All	12675/12690 (100%)	12095 (95%)	541 (4%)	39 (0%)	37	67

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2022	ASP
1	B	2516	ASP
1	D	2022	ASP
1	D	2516	ASP
1	E	27	TYR
1	A	27	TYR
1	A	2516	ASP
1	B	27	TYR

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Mol	Chain	Res	Type
1	B	309	SER
1	C	27	TYR
1	C	309	SER
1	C	2022	ASP
1	C	2516	ASP
1	D	27	TYR
1	E	1730	GLN
1	E	2516	ASP
1	A	309	SER
1	A	1730	GLN
1	B	308	THR
1	B	1730	GLN
1	B	1973	ASN
1	B	2022	ASP
1	C	1730	GLN
1	D	309	SER
1	D	1730	GLN
1	E	308	THR
1	E	309	SER
1	E	2022	ASP
1	A	902	LEU
1	C	308	THR
1	E	1467	THR
1	A	344	ILE
1	B	344	ILE
1	C	344	ILE
1	D	308	THR
1	D	344	ILE
1	E	344	ILE
1	A	308	THR
1	D	902	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2108/2175 (97%)	2104 (100%)	4 (0%)	87	89
1	B	2172/2175 (100%)	2171 (100%)	1 (0%)	100	100
1	C	2172/2175 (100%)	2166 (100%)	6 (0%)	86	87
1	D	2172/2175 (100%)	2169 (100%)	3 (0%)	88	90
1	E	2172/2175 (100%)	2171 (100%)	1 (0%)	100	100
All	All	10796/10875 (99%)	10781 (100%)	15 (0%)	87	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	VAL
1	A	536	ILE
1	A	1117	LEU
1	A	2044	THR
1	B	577	LEU
1	C	1517	THR
1	C	1730	GLN
1	C	1915	MET
1	C	2044	THR
1	C	2306	MET
1	C	2411	ILE
1	D	290	LEU
1	D	1375	ILE
1	D	1915	MET
1	E	961	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	323	ASN
1	A	449	ASN
1	A	507	ASN
1	A	512	ASN
1	A	552	GLN
1	A	695	HIS
1	A	916	GLN

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Mol	Chain	Res	Type
1	A	921	ASN
1	A	1199	HIS
1	A	1259	ASN
1	A	1397	ASN
1	A	1401	HIS
1	A	1532	HIS
1	A	1539	ASN
1	A	1596	ASN
1	A	1661	ASN
1	A	1692	GLN
1	A	1954	GLN
1	A	2032	GLN
1	A	2124	GLN
1	A	2388	GLN
1	A	2483	GLN
1	B	60	ASN
1	B	213	HIS
1	B	323	ASN
1	B	573	GLN
1	B	612	ASN
1	B	695	HIS
1	B	929	GLN
1	B	1199	HIS
1	B	1416	ASN
1	B	1471	ASN
1	B	1562	ASN
1	B	1692	GLN
1	B	1815	GLN
1	B	1877	ASN
1	B	2032	GLN
1	B	2155	GLN
1	B	2240	GLN
1	B	2268	GLN
1	C	60	ASN
1	C	137	HIS
1	C	213	HIS
1	C	345	ASN
1	C	552	GLN
1	C	573	GLN
1	C	612	ASN
1	C	884	HIS
1	C	1065	GLN

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Mol	Chain	Res	Type
1	C	1151	ASN
1	C	1340	GLN
1	C	1388	GLN
1	C	1391	ASN
1	C	1416	ASN
1	C	1459	ASN
1	C	1563	ASN
1	C	1684	ASN
1	C	1688	ASN
1	C	1692	GLN
1	C	1877	ASN
1	C	1992	GLN
1	C	2268	GLN
1	C	2295	GLN
1	C	2318	ASN
1	C	2435	GLN
1	C	2458	ASN
1	D	60	ASN
1	D	213	HIS
1	D	323	ASN
1	D	463	ASN
1	D	507	ASN
1	D	833	GLN
1	D	884	HIS
1	D	1065	GLN
1	D	1340	GLN
1	D	1397	ASN
1	D	1401	HIS
1	D	1532	HIS
1	D	1692	GLN
1	D	1950	GLN
1	D	1992	GLN
1	D	2160	GLN
1	D	2268	GLN
1	E	60	ASN
1	E	137	HIS
1	E	201	GLN
1	E	301	GLN
1	E	466	GLN
1	E	507	ASN
1	E	512	ASN
1	E	865	GLN

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Mol	Chain	Res	Type
1	E	884	HIS
1	E	1356	ASN
1	E	1401	HIS
1	E	1596	ASN
1	E	1661	ASN
1	E	1692	GLN
1	E	1795	ASN
1	E	1815	GLN
1	E	1877	ASN
1	E	2160	GLN
1	E	2373	GLN
1	E	2388	GLN
1	E	2410	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

This section contains visualisations of the EMDB entry EMD-41503. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.