



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:11 PM UTC

PDB ID : 9MLG / pdb_00009mlg
EMDB ID : EMD-48371
Title : Xenorhabdus nematophilus XptA2 State 2, 1181insYWK1183, D1182T mutant
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 4.30 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:

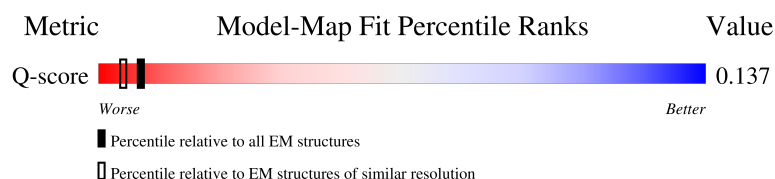
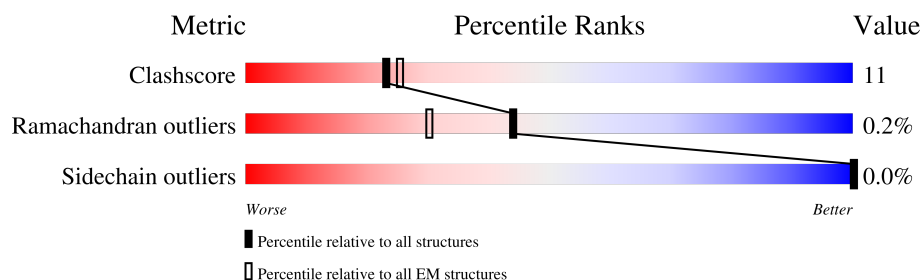
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.30 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	4585 (3.80 - 4.80)

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	2540	
1	B	2540	
1	C	2540	
1	D	2540	

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Mol	Chain	Length	Quality of chain
1	E	2540	14% 75% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100205 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	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	B	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	C	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	D	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	E	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0

There are 625 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	1182	TYR	-	insertion	UNP Q93RN7
A	1183	TRP	-	insertion	UNP Q93RN7
A	1184	LYS	-	insertion	UNP Q93RN7
A	1185	THR	ASP	engineered mutation	UNP Q93RN7
A	1253	LYS	VAL	conflict	UNP Q93RN7
A	1256	SER	PRO	conflict	UNP Q93RN7
A	1260	GLY	ASP	conflict	UNP Q93RN7
A	1261	SER	ASN	conflict	UNP Q93RN7
A	1517	ILE	VAL	conflict	UNP Q93RN7
A	1522	MET	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1880	ASN	TYR	conflict	UNP Q93RN7
A	1883	MET	THR	conflict	UNP Q93RN7
A	1887	ILE	VAL	conflict	UNP Q93RN7
A	1923	THR	ALA	conflict	UNP Q93RN7
A	1946	GLY	VAL	conflict	UNP Q93RN7
A	1950	GLN	HIS	conflict	UNP Q93RN7
A	1962	MET	ALA	conflict	UNP Q93RN7
A	1964	GLY	ASP	conflict	UNP Q93RN7
A	1965	ARG	ASN	conflict	UNP Q93RN7
A	1967	GLY	GLU	conflict	UNP Q93RN7
A	1969	SER	ALA	conflict	UNP Q93RN7
A	1970	LYS	THR	conflict	UNP Q93RN7
A	1971	ASN	GLN	conflict	UNP Q93RN7
A	1972	LEU	PRO	conflict	UNP Q93RN7
A	2031	THR	PRO	conflict	UNP Q93RN7
A	2060	THR	ALA	conflict	UNP Q93RN7
A	2152	LEU	PHE	conflict	UNP Q93RN7
A	2164	VAL	ALA	conflict	UNP Q93RN7
A	2167	ILE	VAL	conflict	UNP Q93RN7
A	2181	LEU	PHE	conflict	UNP Q93RN7
A	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
B	1183	TRP	-	insertion	UNP Q93RN7
B	1184	LYS	-	insertion	UNP Q93RN7
B	1185	THR	ASP	engineered mutation	UNP Q93RN7
B	1253	LYS	VAL	conflict	UNP Q93RN7
B	1256	SER	PRO	conflict	UNP Q93RN7
B	1260	GLY	ASP	conflict	UNP Q93RN7
B	1261	SER	ASN	conflict	UNP Q93RN7
B	1517	ILE	VAL	conflict	UNP Q93RN7
B	1522	MET	VAL	conflict	UNP Q93RN7
B	1880	ASN	TYR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1883	MET	THR	conflict	UNP Q93RN7
B	1887	ILE	VAL	conflict	UNP Q93RN7
B	1923	THR	ALA	conflict	UNP Q93RN7
B	1946	GLY	VAL	conflict	UNP Q93RN7
B	1950	GLN	HIS	conflict	UNP Q93RN7
B	1962	MET	ALA	conflict	UNP Q93RN7
B	1964	GLY	ASP	conflict	UNP Q93RN7
B	1965	ARG	ASN	conflict	UNP Q93RN7
B	1967	GLY	GLU	conflict	UNP Q93RN7
B	1969	SER	ALA	conflict	UNP Q93RN7
B	1970	LYS	THR	conflict	UNP Q93RN7
B	1971	ASN	GLN	conflict	UNP Q93RN7
B	1972	LEU	PRO	conflict	UNP Q93RN7
B	2031	THR	PRO	conflict	UNP Q93RN7
B	2060	THR	ALA	conflict	UNP Q93RN7
B	2152	LEU	PHE	conflict	UNP Q93RN7
B	2164	VAL	ALA	conflict	UNP Q93RN7
B	2167	ILE	VAL	conflict	UNP Q93RN7
B	2181	LEU	PHE	conflict	UNP Q93RN7
B	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
C	1183	TRP	-	insertion	UNP Q93RN7
C	1184	LYS	-	insertion	UNP Q93RN7
C	1185	THR	ASP	engineered mutation	UNP Q93RN7
C	1253	LYS	VAL	conflict	UNP Q93RN7
C	1256	SER	PRO	conflict	UNP Q93RN7
C	1260	GLY	ASP	conflict	UNP Q93RN7
C	1261	SER	ASN	conflict	UNP Q93RN7
C	1517	ILE	VAL	conflict	UNP Q93RN7
C	1522	MET	VAL	conflict	UNP Q93RN7
C	1880	ASN	TYR	conflict	UNP Q93RN7
C	1883	MET	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1887	ILE	VAL	conflict	UNP Q93RN7
C	1923	THR	ALA	conflict	UNP Q93RN7
C	1946	GLY	VAL	conflict	UNP Q93RN7
C	1950	GLN	HIS	conflict	UNP Q93RN7
C	1962	MET	ALA	conflict	UNP Q93RN7
C	1964	GLY	ASP	conflict	UNP Q93RN7
C	1965	ARG	ASN	conflict	UNP Q93RN7
C	1967	GLY	GLU	conflict	UNP Q93RN7
C	1969	SER	ALA	conflict	UNP Q93RN7
C	1970	LYS	THR	conflict	UNP Q93RN7
C	1971	ASN	GLN	conflict	UNP Q93RN7
C	1972	LEU	PRO	conflict	UNP Q93RN7
C	2031	THR	PRO	conflict	UNP Q93RN7
C	2060	THR	ALA	conflict	UNP Q93RN7
C	2152	LEU	PHE	conflict	UNP Q93RN7
C	2164	VAL	ALA	conflict	UNP Q93RN7
C	2167	ILE	VAL	conflict	UNP Q93RN7
C	2181	LEU	PHE	conflict	UNP Q93RN7
C	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
D	1183	TRP	-	insertion	UNP Q93RN7
D	1184	LYS	-	insertion	UNP Q93RN7
D	1185	THR	ASP	engineered mutation	UNP Q93RN7
D	1253	LYS	VAL	conflict	UNP Q93RN7
D	1256	SER	PRO	conflict	UNP Q93RN7
D	1260	GLY	ASP	conflict	UNP Q93RN7
D	1261	SER	ASN	conflict	UNP Q93RN7
D	1517	ILE	VAL	conflict	UNP Q93RN7
D	1522	MET	VAL	conflict	UNP Q93RN7
D	1880	ASN	TYR	conflict	UNP Q93RN7
D	1883	MET	THR	conflict	UNP Q93RN7
D	1887	ILE	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1923	THR	ALA	conflict	UNP Q93RN7
D	1946	GLY	VAL	conflict	UNP Q93RN7
D	1950	GLN	HIS	conflict	UNP Q93RN7
D	1962	MET	ALA	conflict	UNP Q93RN7
D	1964	GLY	ASP	conflict	UNP Q93RN7
D	1965	ARG	ASN	conflict	UNP Q93RN7
D	1967	GLY	GLU	conflict	UNP Q93RN7
D	1969	SER	ALA	conflict	UNP Q93RN7
D	1970	LYS	THR	conflict	UNP Q93RN7
D	1971	ASN	GLN	conflict	UNP Q93RN7
D	1972	LEU	PRO	conflict	UNP Q93RN7
D	2031	THR	PRO	conflict	UNP Q93RN7
D	2060	THR	ALA	conflict	UNP Q93RN7
D	2152	LEU	PHE	conflict	UNP Q93RN7
D	2164	VAL	ALA	conflict	UNP Q93RN7
D	2167	ILE	VAL	conflict	UNP Q93RN7
D	2181	LEU	PHE	conflict	UNP Q93RN7
D	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
E	1183	TRP	-	insertion	UNP Q93RN7
E	1184	LYS	-	insertion	UNP Q93RN7
E	1185	THR	ASP	engineered mutation	UNP Q93RN7
E	1253	LYS	VAL	conflict	UNP Q93RN7
E	1256	SER	PRO	conflict	UNP Q93RN7
E	1260	GLY	ASP	conflict	UNP Q93RN7
E	1261	SER	ASN	conflict	UNP Q93RN7
E	1517	ILE	VAL	conflict	UNP Q93RN7
E	1522	MET	VAL	conflict	UNP Q93RN7
E	1880	ASN	TYR	conflict	UNP Q93RN7
E	1883	MET	THR	conflict	UNP Q93RN7
E	1887	ILE	VAL	conflict	UNP Q93RN7
E	1923	THR	ALA	conflict	UNP Q93RN7

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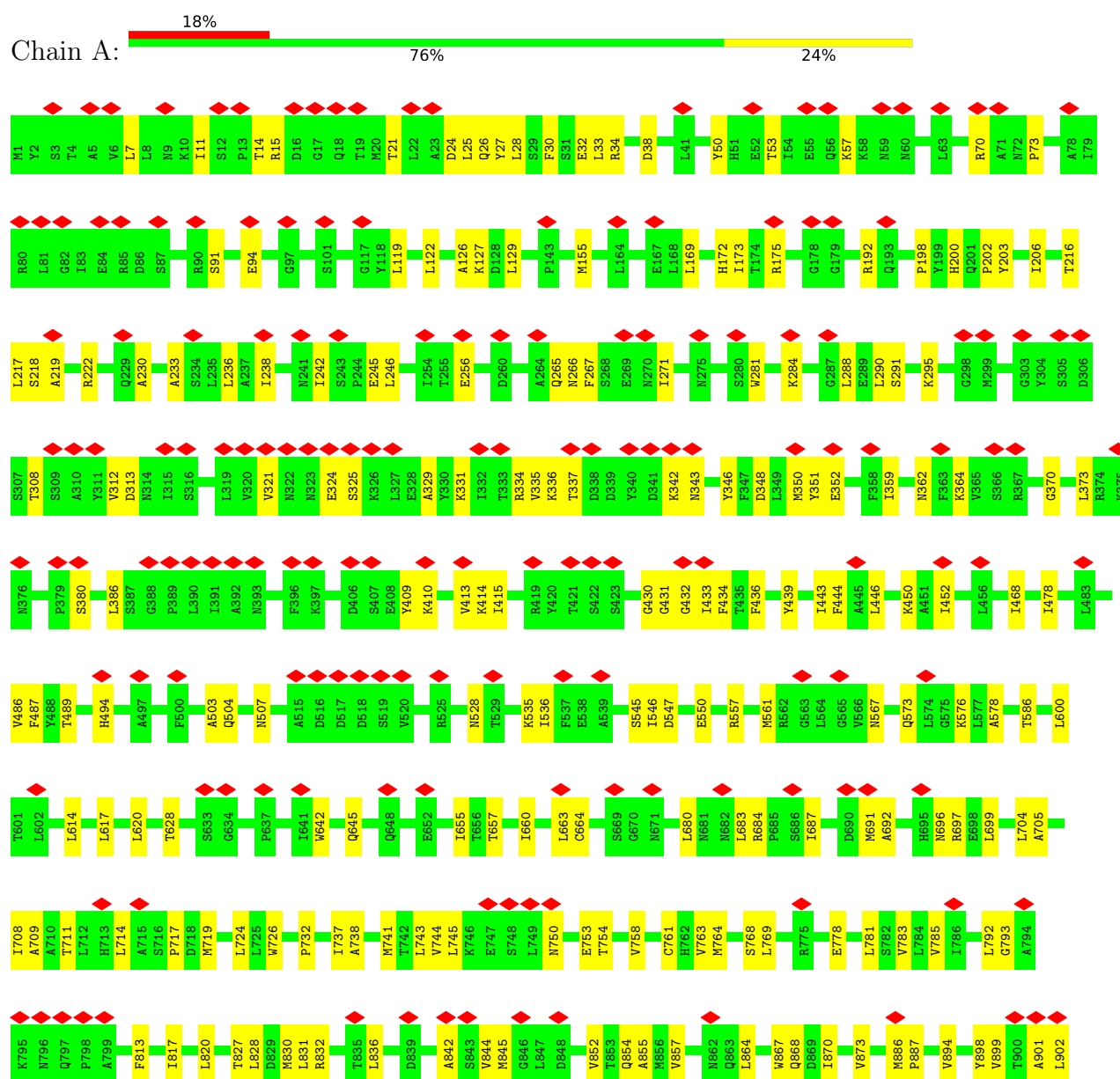
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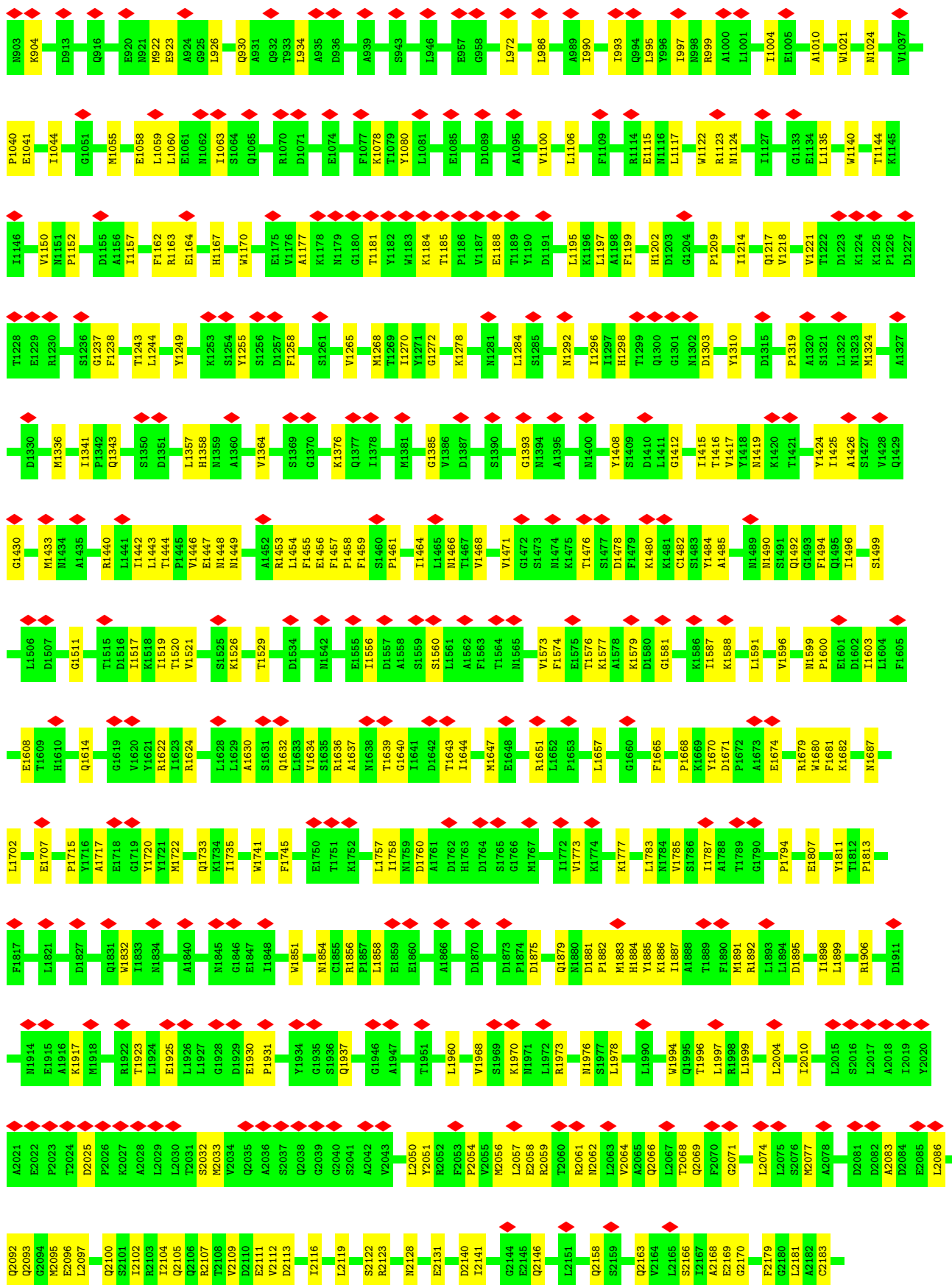
Chain	Residue	Modelled	Actual	Comment	Reference
E	1946	GLY	VAL	conflict	UNP Q93RN7
E	1950	GLN	HIS	conflict	UNP Q93RN7
E	1962	MET	ALA	conflict	UNP Q93RN7
E	1964	GLY	ASP	conflict	UNP Q93RN7
E	1965	ARG	ASN	conflict	UNP Q93RN7
E	1967	GLY	GLU	conflict	UNP Q93RN7
E	1969	SER	ALA	conflict	UNP Q93RN7
E	1970	LYS	THR	conflict	UNP Q93RN7
E	1971	ASN	GLN	conflict	UNP Q93RN7
E	1972	LEU	PRO	conflict	UNP Q93RN7
E	2031	THR	PRO	conflict	UNP Q93RN7
E	2060	THR	ALA	conflict	UNP Q93RN7
E	2152	LEU	PHE	conflict	UNP Q93RN7
E	2164	VAL	ALA	conflict	UNP Q93RN7
E	2167	ILE	VAL	conflict	UNP Q93RN7
E	2181	LEU	PHE	conflict	UNP Q93RN7
E	2433	LEU	PHE	conflict	UNP Q93RN7

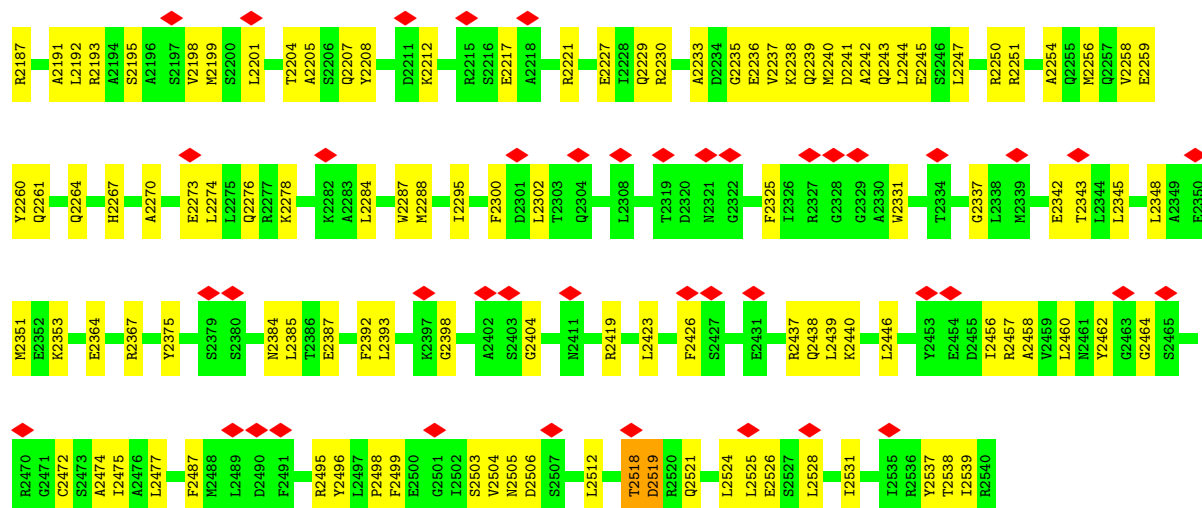
3 Residue-property plots

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.

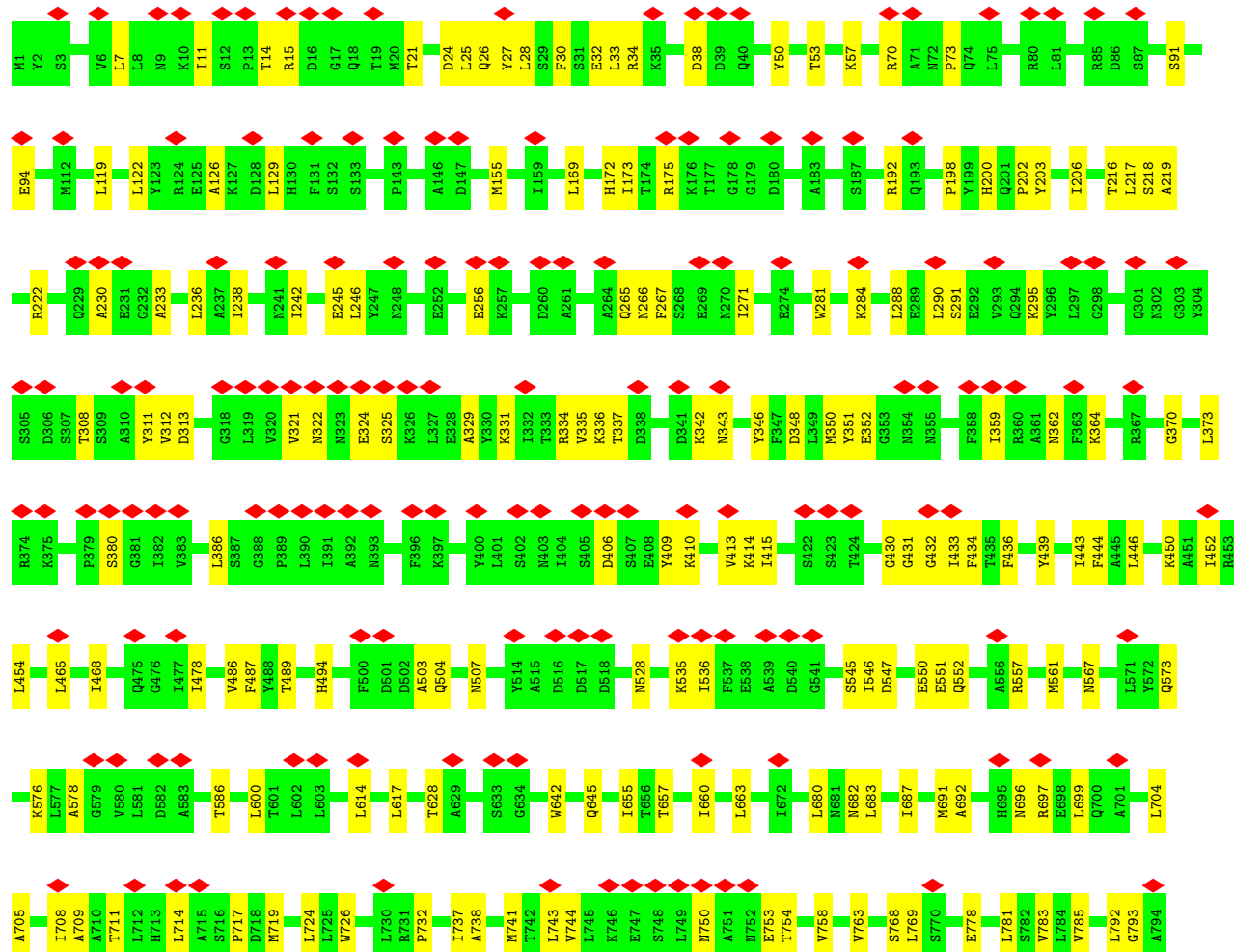
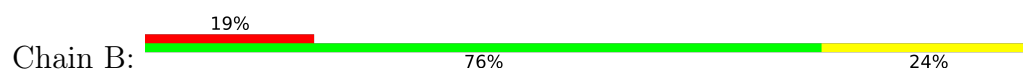
• Molecule 1: XptA2 protein



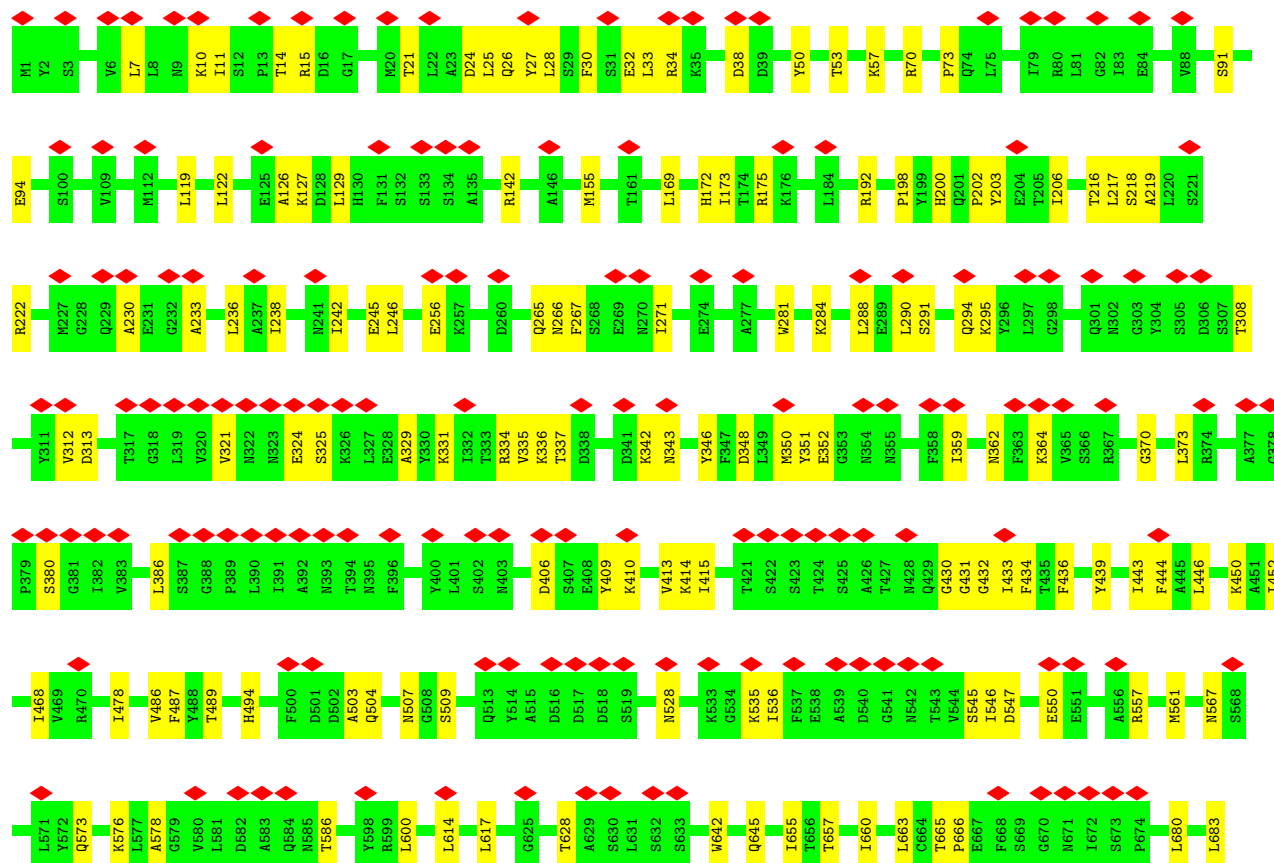


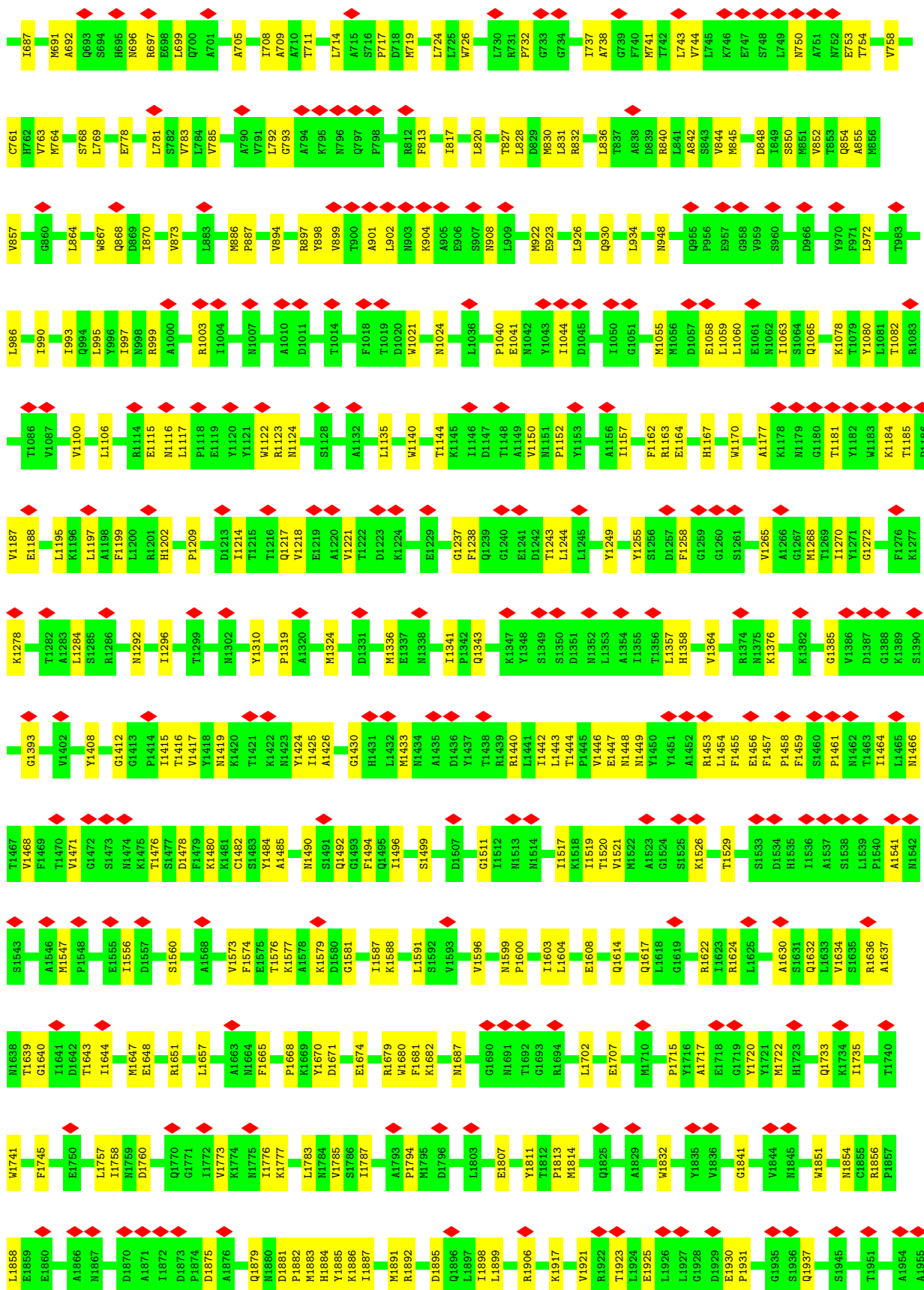


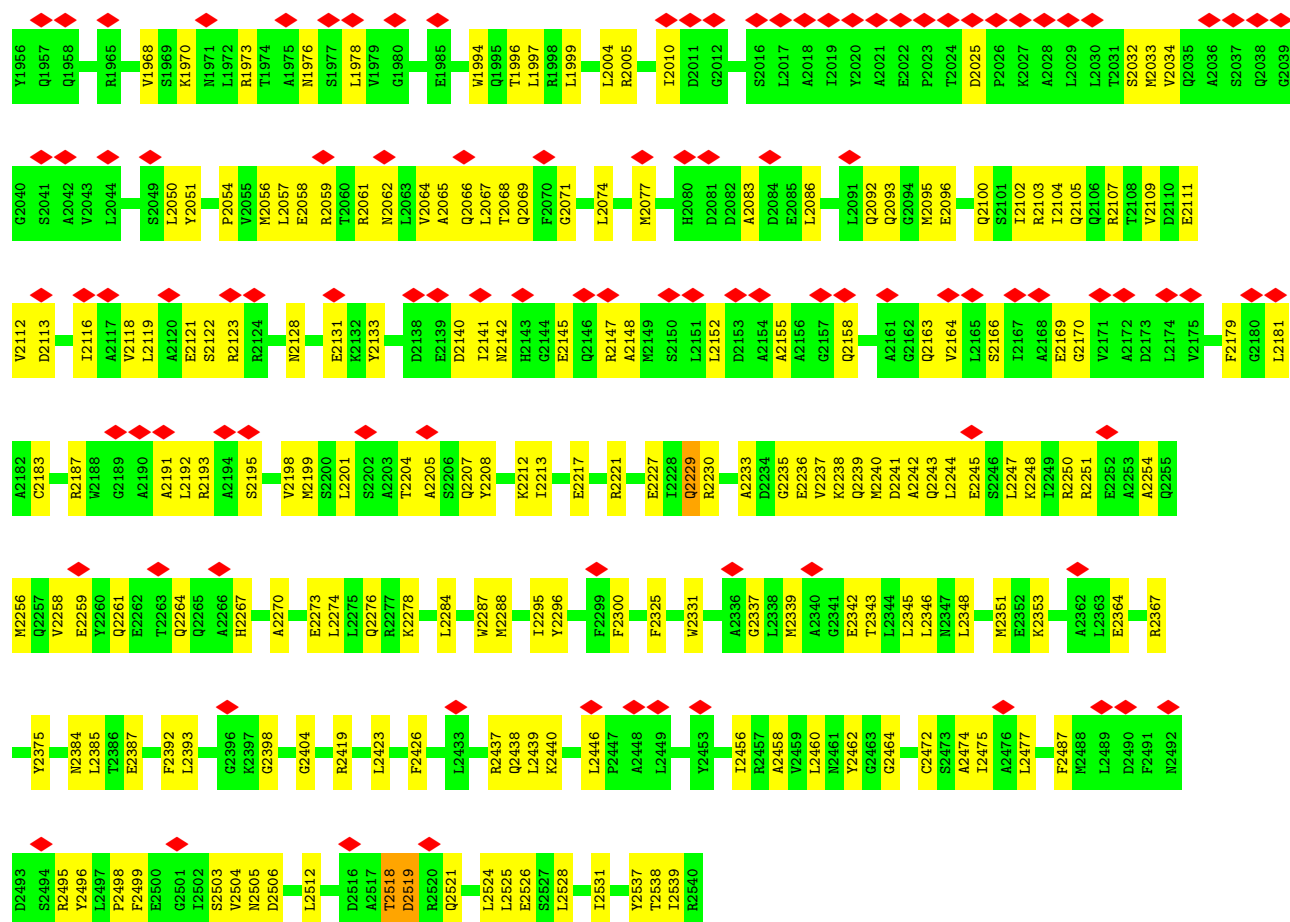
• Molecule 1: XptA2 protein



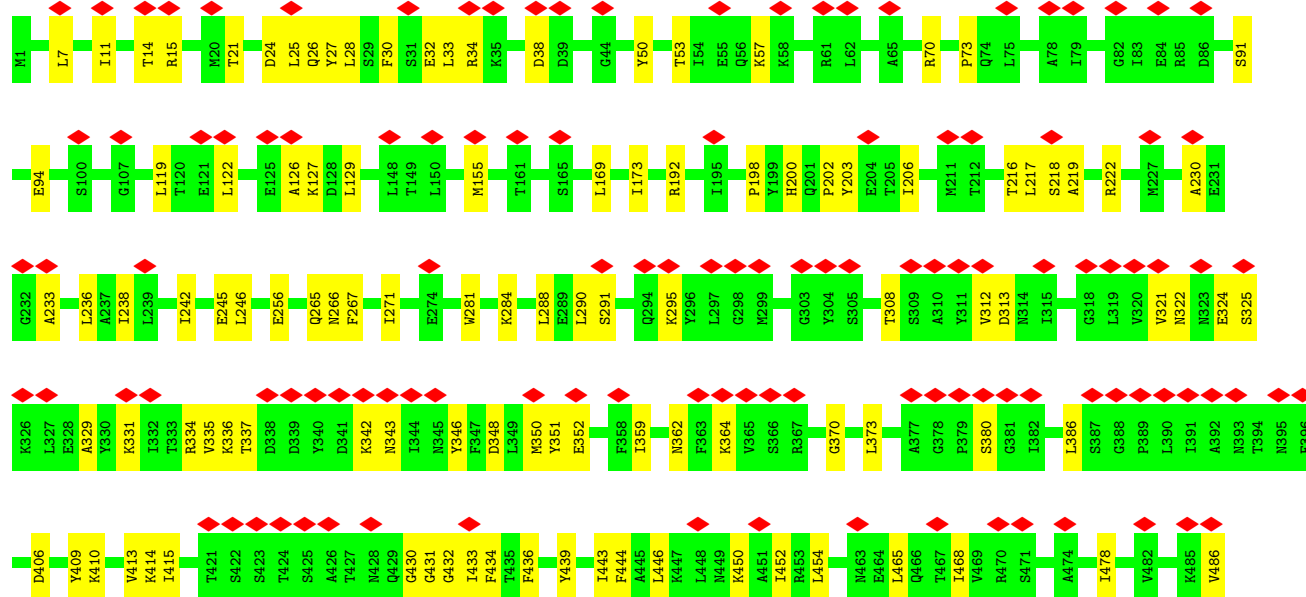
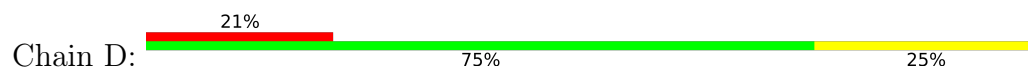


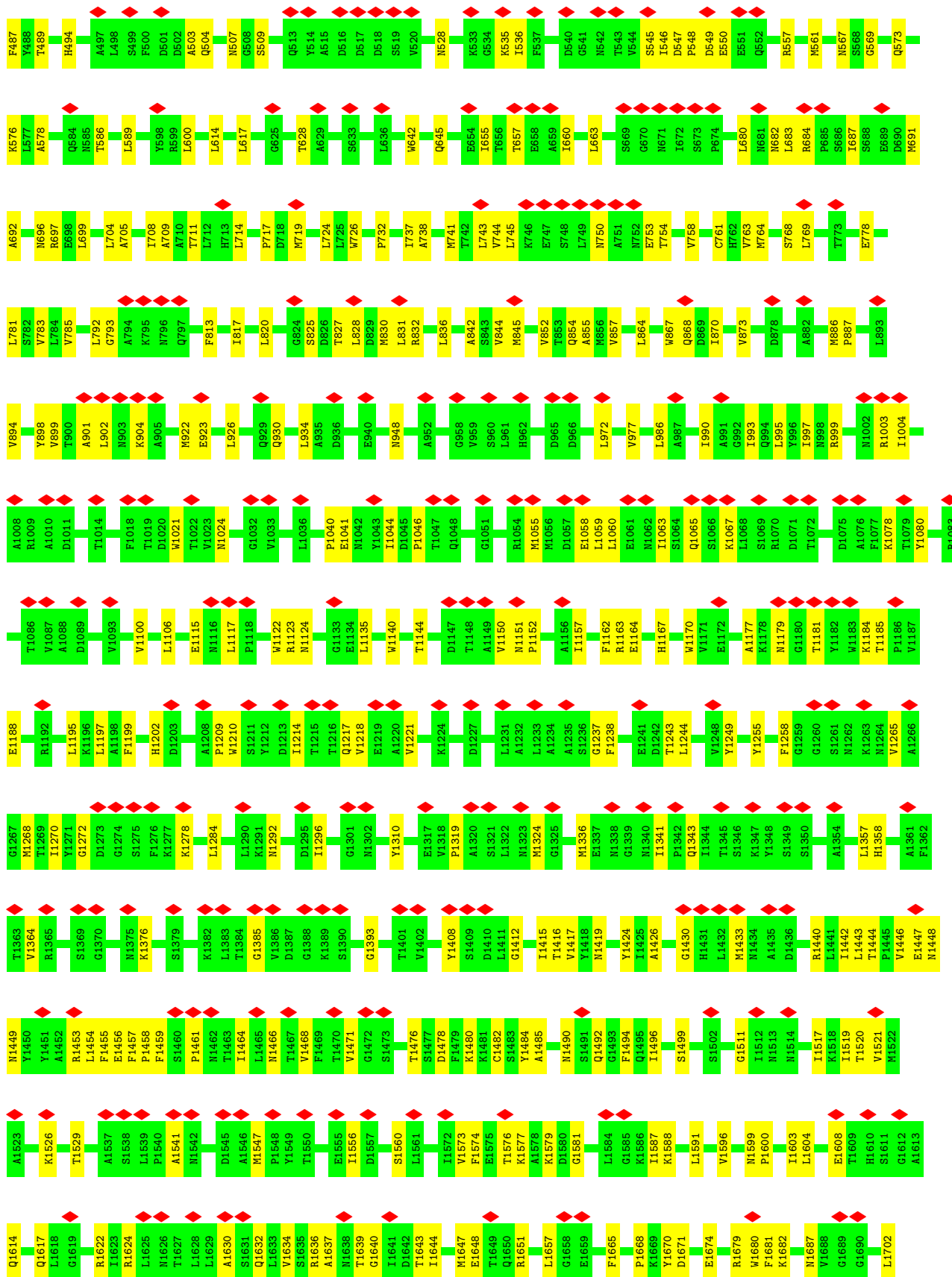


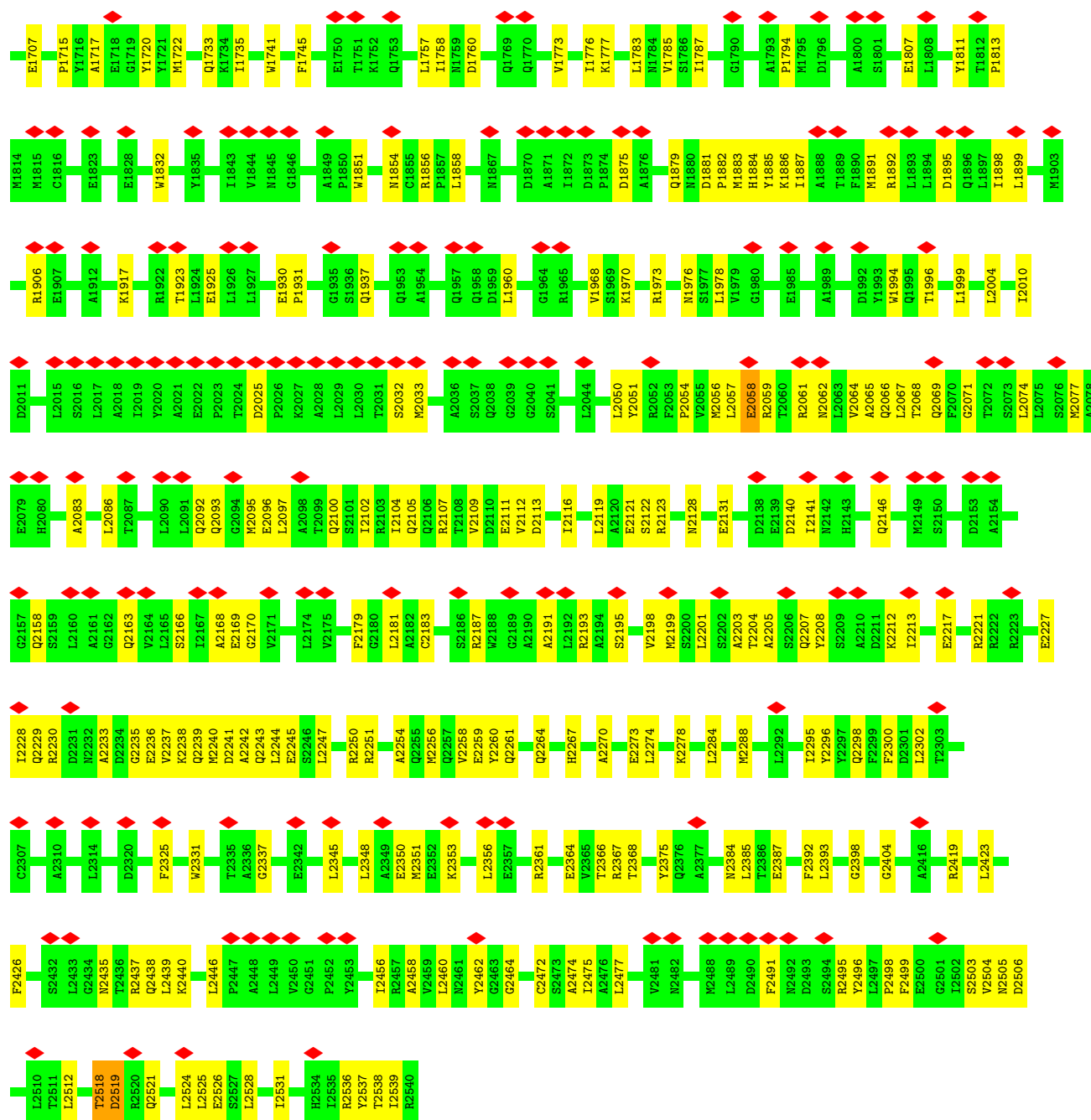




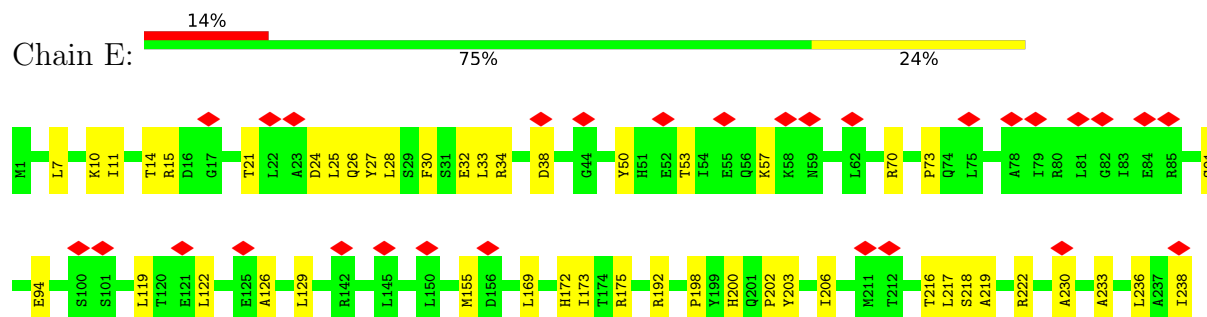
• Molecule 1: XptA2 protein

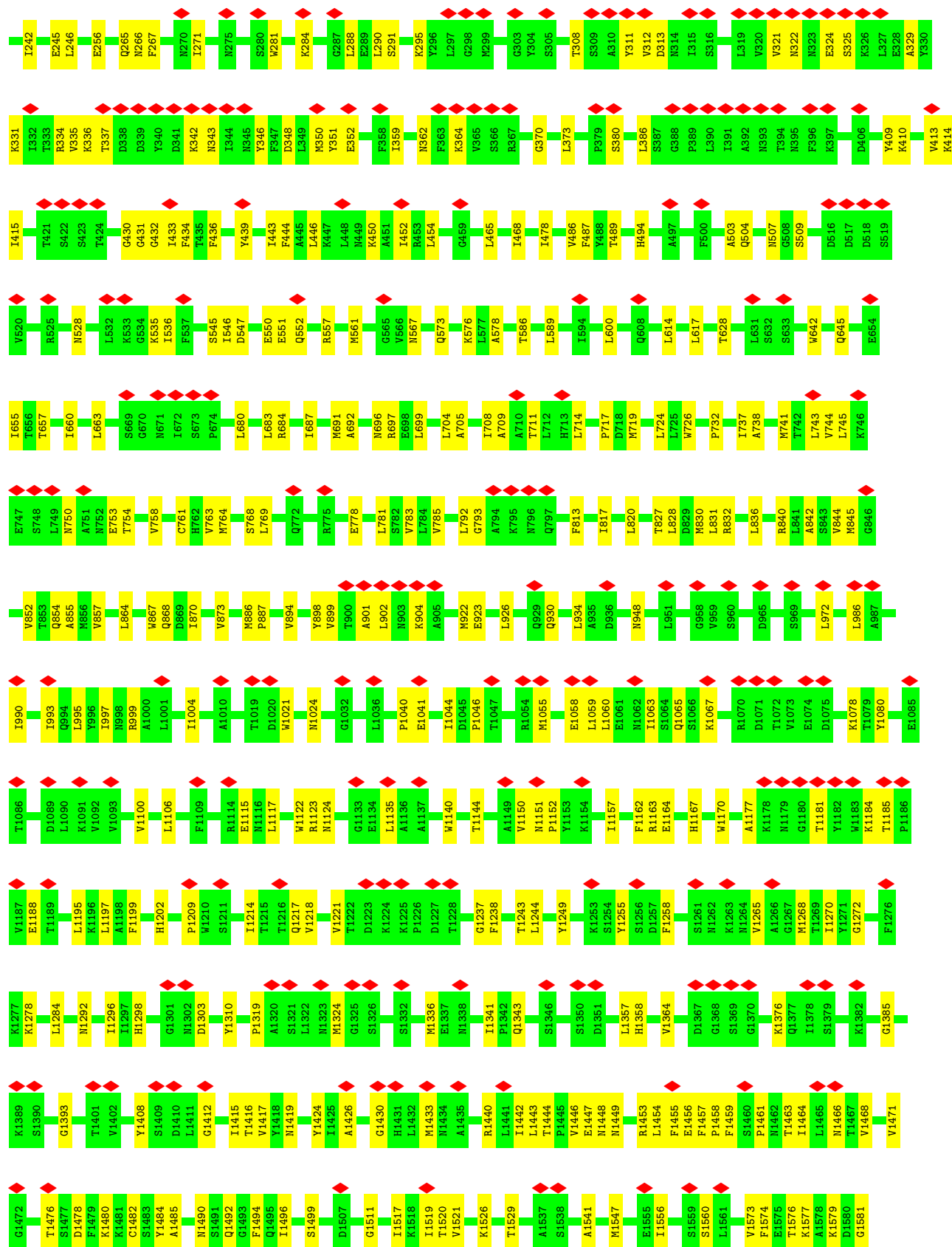






• Molecule 1: XptA2 protein





V2504	G2398	A2270	S1915	L2091	L2017	A1888	S1765	D1671	I1587
N2505	G2404	E2273	V2198	Q2092	A2018	T1889	I1787	E1674	K1588
D2506	M2199	L2274	M2199	Q2093	I2019	F1890	G1790	R1679	L1591
L2512	R2419	K2278	S2200	W2095	Y2020	M1891	Y1791	F1681	V1596
T2518	L2423	L2284	L2201	L2097	A2021	R1892	S1792	K1682	
D2519	F2426	L2296	T2204	Q2100	E2022	L1893	A1793		
R2520	S2427	M2288	A2205	S2101	P2023	D1894	P1794		
Q2521	D2428	Y2296	S2206	I2102	T2024	I1898	S1801	N1687	M1599
L2524	L2433	F2300	Y2208	R2103	D2025	L1899	Y1804	M1701	P1600
L2525	Q2438	D2301	A2210	T2104	K2027	M1903	E1807	L1702	E1601
E2526	D2302	L2302	D2211	Q2105	A2028	A1904	L1908	E1707	D1602
L2528	G2322	K2212	K2212	Q2106	L2029	Y1905	E1809	T1708	I1603
	F2325	I2213	I2213	R2107	L2030	R1906	Y1811	S1709	E1608
L2531	F2326	S2214	V2109	Q2110	T2031	E1907	T1812	H1610	H1610
	L2326	E2217	E2111	E2111	S2032		P1813	Q1614	Q1614
Y2537	R2327	R2221	D2112	D2113	M2033		G1816	A1717	Q1617
T2538	W2331	E2227	I2116	I2116	V2034	K1917	E1718	Y1716	
I2539	Q2337	I2228	L2119	L2119	Q2035	R1922	G1719	E1716	
R2540	L2338	Q2229	S2122	S2122	A2036	T1923	Y1720	I1623	R1622
	M2339	R2230	R2123	R2123	Q2038	I1924	Y1721	Y1721	R1624
	E2342	A2233	D2140	D2140	G2039	E1925	M1722	Q1733	
	T2343	D2234	T2141	T2141	G2040	L1926	E1828	I1628	L1629
	L2345	G2235	R2147	R2147	S2041	D1929	W1832	L1629	L1629
	L2346	E2236	Q2158	Q2158	E1930	E1930	I1833	A1630	A1630
	L2347	V2237	Q2163	Q2163	P1931	P1931	M1834	S1431	S1431
	L2348	K2238	Q2166	Q2166			I1843	L1633	L1633
	M2351	Q2239	S2166	S2166	G2046		V1844	V1634	V1634
	E2352	M2240	E2169	E2169	L2050	A1947	V1845	S1635	S1635
	K2353	A2242	E2170	E2170	P2054	V1968	G1846	A1637	A1637
	L2356	L2244	G2170	G2170	M2055	S1989	E1847	M1638	M1638
	F2357	E2245	L2174	L2174	L2057	I1970	I1848	T1639	T1639
	E2364	L2247	F2179	F2179	E2058	N1971	W1851	G1640	G1640
	R2367	R2250	Q2180	Q2180	R2059	N1972	N1854	T1643	T1643
	Y2375	R2251	A2181	A2181	T2060	R1973	C1855	I1644	I1644
	S2379	A2254	Q2182	Q2182	N2062	S1977	R1856	M1647	M1647
	N2384	M2256	C2183	C2183	N2063	L1978	P1857	E1648	E1648
	L2385	Q2257	R2187	R2187	A2065	Q1995	L1858	R1651	R1651
	T2386	V2258	Q2188	Q2188	Q2066	T1996	D1870	L1652	L1652
	E2387	E2259	Q2189	Q2189	L2067	Q1997	A1871	M1767	M1767
	F2392	Q2261	A2190	A2190	Q2069	L1998	D1875	T1768	T1768
	L2393	Q2264	L2191	L2191	F2070	L1999	Q1879	Q1769	Q1769
		H2267	R2192	R2192	G2071	N1880	V1773	I1772	I1772
			R2193	R2193	L2074	D1881	K1777	V1773	V1773
			A2194	A2194	M2077	P1882			
					A2083	M1883			
					L2086	H1884			
					L2090	Y1885			
						K1886			
						I1887			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.069	Depositor
Minimum map value	-0.470	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	473.796, 473.796, 473.796	wwPDB
Map dimensions	246, 246, 246	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.926, 1.926, 1.926	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	0.14	0/20450	0.40	2/27765 (0.0%)
1	B	0.14	0/20450	0.40	4/27765 (0.0%)
1	C	0.14	0/20450	0.40	2/27765 (0.0%)
1	D	0.14	0/20450	0.40	4/27765 (0.0%)
1	E	0.14	0/20450	0.40	2/27765 (0.0%)
All	All	0.14	0/102250	0.40	14/138825 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2518	THR	CA-C-N	9.52	138.83	121.70
1	D	2518	THR	C-N-CA	9.52	138.83	121.70
1	B	2518	THR	CA-C-N	9.50	138.80	121.70
1	B	2518	THR	C-N-CA	9.50	138.80	121.70
1	C	2518	THR	CA-C-N	9.49	138.79	121.70
1	C	2518	THR	C-N-CA	9.49	138.79	121.70
1	A	2518	THR	CA-C-N	9.48	138.77	121.70
1	A	2518	THR	C-N-CA	9.48	138.77	121.70
1	E	2518	THR	CA-C-N	9.47	138.75	121.70
1	E	2518	THR	C-N-CA	9.47	138.75	121.70
1	D	2058	GLU	CA-C-N	-5.03	112.34	121.14
1	D	2058	GLU	C-N-CA	-5.03	112.34	121.14
1	B	2058	GLU	CA-C-N	-5.01	112.37	121.14
1	B	2058	GLU	C-N-CA	-5.01	112.37	121.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20041	0	19627	443	0
1	B	20041	0	19627	454	0
1	C	20041	0	19627	493	0
1	D	20041	0	19627	509	0
1	E	20041	0	19627	463	0
All	All	100205	0	98135	2194	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 11.

All (2194) 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:2518:THR:H	1:C:2519:ASP:HB2	1.22	1.04
1:D:2518:THR:H	1:D:2519:ASP:HB2	1.22	1.04
1:B:2518:THR:H	1:B:2519:ASP:HB2	1.22	1.00
1:A:2518:THR:H	1:A:2519:ASP:HB2	1.22	0.99
1:E:2518:THR:H	1:E:2519:ASP:HB2	1.22	0.99
1:C:2122:SER:HA	1:D:2239:GLN:HE22	1.27	0.99
1:B:2169:GLU:HG2	1:C:2192:LEU:HD11	1.45	0.96
1:C:2158:GLN:O	1:D:2199:MET:HE1	1.70	0.91
1:A:1185:THR:HG23	1:B:1181:THR:HA	1.51	0.90
1:E:1443:LEU:HB2	1:E:1455:PHE:HB2	1.55	0.89
1:C:1443:LEU:HB2	1:C:1455:PHE:HB2	1.55	0.88
1:B:1443:LEU:HB2	1:B:1455:PHE:HB2	1.55	0.88
1:D:1443:LEU:HB2	1:D:1455:PHE:HB2	1.55	0.87
1:A:1181:THR:HA	1:E:1185:THR:HG23	1.56	0.86
1:A:1443:LEU:HB2	1:A:1455:PHE:HB2	1.55	0.86
1:D:2158:GLN:HE21	1:E:2199:MET:HE2	1.43	0.84
1:B:1078:LYS:HE2	1:C:1202:HIS:HB3	1.59	0.82
1:C:334:ARG:HG3	1:C:415:ILE:HG13	1.61	0.82
1:D:334:ARG:HG3	1:D:415:ILE:HG13	1.61	0.82
1:A:2122:SER:HA	1:B:2239:GLN:HE22	1.43	0.82
1:D:719:MET:HE3	1:D:778:GLU:HG3	1.62	0.82
1:A:334:ARG:HG3	1:A:415:ILE:HG13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:MET:HE3	1:C:778:GLU:HG3	1.62	0.81
1:E:719:MET:HE3	1:E:778:GLU:HG3	1.62	0.81
1:B:719:MET:HE3	1:B:778:GLU:HG3	1.62	0.81
1:A:683:LEU:HD23	1:A:744:VAL:HG11	1.62	0.81
1:B:683:LEU:HD23	1:B:744:VAL:HG11	1.62	0.81
1:E:334:ARG:HG3	1:E:415:ILE:HG13	1.61	0.81
1:D:683:LEU:HD23	1:D:744:VAL:HG11	1.62	0.81
1:A:719:MET:HE3	1:A:778:GLU:HG3	1.62	0.80
1:B:334:ARG:HG3	1:B:415:ILE:HG13	1.61	0.80
1:C:2104:ILE:HG12	1:D:2256:MET:SD	2.21	0.80
1:C:683:LEU:HD23	1:C:744:VAL:HG11	1.62	0.79
1:E:683:LEU:HD23	1:E:744:VAL:HG11	1.62	0.79
1:C:1925:GLU:HG2	1:D:1004:ILE:HD13	1.64	0.78
1:D:1185:THR:HG23	1:E:1181:THR:HA	1.67	0.75
1:C:2122:SER:HA	1:D:2239:GLN:NE2	2.02	0.74
1:E:155:MET:HB3	1:E:986:LEU:HD12	1.70	0.74
1:A:155:MET:HB3	1:A:986:LEU:HD12	1.70	0.74
1:D:1917:LYS:HE2	1:D:2004:LEU:HB3	1.70	0.74
1:D:155:MET:HB3	1:D:986:LEU:HD12	1.70	0.73
1:D:1858:LEU:HD12	1:D:1886:LYS:HG3	1.71	0.73
1:E:1858:LEU:HD12	1:E:1886:LYS:HG3	1.71	0.73
1:B:1135:LEU:HD13	1:B:1140:TRP:HE1	1.54	0.73
1:D:1078:LYS:HE2	1:E:1202:HIS:HB3	1.69	0.73
1:B:155:MET:HB3	1:B:986:LEU:HD12	1.70	0.73
1:C:1858:LEU:HD12	1:C:1886:LYS:HG3	1.71	0.73
1:D:2122:SER:HA	1:E:2239:GLN:HE22	1.54	0.72
1:C:1135:LEU:HD13	1:C:1140:TRP:HE1	1.54	0.72
1:C:155:MET:HB3	1:C:986:LEU:HD12	1.70	0.72
1:C:1917:LYS:HE2	1:C:2004:LEU:HB3	1.70	0.72
1:D:1517:ILE:HG12	1:D:1576:THR:HG23	1.72	0.72
1:E:2264:GLN:HA	1:E:2267:HIS:CE1	2.25	0.72
1:A:1917:LYS:HE2	1:A:2004:LEU:HB3	1.70	0.72
1:A:1858:LEU:HD12	1:A:1886:LYS:HG3	1.71	0.72
1:A:2264:GLN:HA	1:A:2267:HIS:CE1	2.25	0.72
1:C:2122:SER:CA	1:D:2239:GLN:HE22	2.02	0.72
1:D:2518:THR:N	1:D:2519:ASP:HB2	2.03	0.72
1:E:1258:PHE:HB3	1:E:1284:LEU:HG	1.72	0.72
1:B:325:SER:HB2	1:B:1492:GLN:HB3	1.72	0.72
1:C:1517:ILE:HG12	1:C:1576:THR:HG23	1.72	0.72
1:C:2264:GLN:HA	1:C:2267:HIS:CE1	2.25	0.72
1:D:2435:ASN:HD21	1:E:2470:ARG:HH12	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1258:PHE:HB3	1:D:1284:LEU:HG	1.72	0.72
1:D:1135:LEU:HD13	1:D:1140:TRP:HE1	1.54	0.71
1:D:2264:GLN:HA	1:D:2267:HIS:CE1	2.25	0.71
1:E:1517:ILE:HG12	1:E:1576:THR:HG23	1.72	0.71
1:B:1858:LEU:HD12	1:B:1886:LYS:HG3	1.71	0.71
1:C:1185:THR:HG23	1:D:1181:THR:HA	1.72	0.71
1:B:2247:LEU:HD23	1:B:2250:ARG:HE	1.56	0.71
1:C:325:SER:HB2	1:C:1492:GLN:HB3	1.72	0.71
1:C:2163:GLN:HG3	1:C:2198:VAL:HB	1.73	0.71
1:D:2163:GLN:HG3	1:D:2198:VAL:HB	1.73	0.71
1:E:2163:GLN:HG3	1:E:2198:VAL:HB	1.73	0.71
1:A:1135:LEU:HD13	1:A:1140:TRP:HE1	1.54	0.71
1:B:1917:LYS:HE2	1:B:2004:LEU:HB3	1.70	0.71
1:E:1917:LYS:HE2	1:E:2004:LEU:HB3	1.70	0.71
1:E:2123:ARG:HH12	1:E:2237:VAL:HG13	1.56	0.71
1:A:325:SER:HB2	1:A:1492:GLN:HB3	1.72	0.71
1:A:2158:GLN:HE21	1:B:2199:MET:HE2	1.56	0.71
1:E:1162:PHE:CG	1:E:1244:LEU:HD21	2.26	0.71
1:E:1135:LEU:HD13	1:E:1140:TRP:HE1	1.54	0.71
1:B:2518:THR:N	1:B:2519:ASP:HB2	2.03	0.71
1:C:2247:LEU:HD23	1:C:2250:ARG:HE	1.56	0.71
1:E:2247:LEU:HD23	1:E:2250:ARG:HE	1.56	0.71
1:A:1258:PHE:HB3	1:A:1284:LEU:HG	1.72	0.71
1:A:2163:GLN:HG3	1:A:2198:VAL:HB	1.73	0.71
1:E:325:SER:HB2	1:E:1492:GLN:HB3	1.72	0.71
1:B:2264:GLN:HA	1:B:2267:HIS:CE1	2.25	0.70
1:A:2247:LEU:HD23	1:A:2250:ARG:HE	1.56	0.70
1:B:2163:GLN:HG3	1:B:2198:VAL:HB	1.73	0.70
1:C:1162:PHE:CG	1:C:1244:LEU:HD21	2.26	0.70
1:D:325:SER:HB2	1:D:1492:GLN:HB3	1.72	0.70
1:C:528:ASN:HD21	1:C:536:ILE:HG21	1.56	0.70
1:D:528:ASN:HD21	1:D:536:ILE:HG21	1.56	0.70
1:D:2247:LEU:HD23	1:D:2250:ARG:HE	1.56	0.70
1:C:1258:PHE:HB3	1:C:1284:LEU:HG	1.72	0.70
1:D:2123:ARG:HH12	1:D:2237:VAL:HG13	1.56	0.70
1:A:2123:ARG:HH12	1:A:2237:VAL:HG13	1.55	0.70
1:A:1517:ILE:HG12	1:A:1576:THR:HG23	1.72	0.70
1:B:1162:PHE:CG	1:B:1244:LEU:HD21	2.26	0.70
1:B:1258:PHE:HB3	1:B:1284:LEU:HG	1.72	0.70
1:A:1162:PHE:CG	1:A:1244:LEU:HD21	2.26	0.70
1:B:1517:ILE:HG12	1:B:1576:THR:HG23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ASN:HD21	1:A:536:ILE:HG21	1.56	0.70
1:B:1634:VAL:HG22	1:C:1202:HIS:CE1	2.26	0.70
1:D:1162:PHE:CG	1:D:1244:LEU:HD21	2.26	0.69
1:A:2212:LYS:HZ1	1:D:1065:GLN:HG3	1.57	0.69
1:B:528:ASN:HD21	1:B:536:ILE:HG21	1.56	0.69
1:B:2123:ARG:HH12	1:B:2237:VAL:HG13	1.55	0.69
1:C:1082:THR:OG1	1:D:1202:HIS:HB2	1.92	0.69
1:C:2123:ARG:HH12	1:C:2237:VAL:HG13	1.56	0.69
1:A:26:GLN:HB3	1:A:27:TYR:HA	1.75	0.69
1:A:2295:ILE:HG23	1:E:2346:LEU:HD22	1.73	0.69
1:C:2287:TRP:HH2	1:D:682:ASN:HD21	1.40	0.69
1:B:26:GLN:HB3	1:B:27:TYR:HA	1.75	0.69
1:E:528:ASN:HD21	1:E:536:ILE:HG21	1.56	0.68
1:E:26:GLN:HB3	1:E:27:TYR:HA	1.75	0.68
1:D:2356:LEU:HD13	1:E:2059:ARG:HH21	1.58	0.68
1:E:2518:THR:N	1:E:2519:ASP:HB2	2.03	0.68
1:A:2518:THR:N	1:A:2519:ASP:HB2	2.03	0.68
1:E:236:LEU:HD13	1:E:487:PHE:HB2	1.76	0.68
1:C:2518:THR:N	1:C:2519:ASP:HB2	2.03	0.68
1:C:2181:LEU:HD21	1:D:2181:LEU:HD13	1.76	0.68
1:D:236:LEU:HD13	1:D:487:PHE:HB2	1.76	0.68
1:C:236:LEU:HD13	1:C:487:PHE:HB2	1.76	0.67
1:A:2325:PHE:HB2	1:A:2351:MET:HE2	1.76	0.67
1:C:26:GLN:HB3	1:C:27:TYR:HA	1.75	0.67
1:E:2325:PHE:HB2	1:E:2351:MET:HE2	1.76	0.67
1:D:26:GLN:HB3	1:D:27:TYR:HA	1.75	0.67
1:D:336:LYS:HD3	1:D:415:ILE:HG22	1.77	0.67
1:D:1937:GLN:HE21	1:E:290:LEU:HD21	1.59	0.67
1:A:236:LEU:HD13	1:A:487:PHE:HB2	1.76	0.67
1:B:2325:PHE:HB2	1:B:2351:MET:HE2	1.76	0.67
1:D:2353:LYS:HD2	1:E:2302:LEU:HD22	1.77	0.67
1:C:2158:GLN:HE21	1:D:2199:MET:HB2	1.60	0.67
1:C:2325:PHE:HB2	1:C:2351:MET:HE2	1.76	0.66
1:B:836:LEU:HB3	1:B:864:LEU:HD11	1.78	0.66
1:E:321:VAL:HG23	1:E:352:GLU:HG2	1.78	0.66
1:C:836:LEU:HB3	1:C:864:LEU:HD11	1.78	0.66
1:C:2353:LYS:HD2	1:D:2302:LEU:HD22	1.78	0.66
1:A:336:LYS:HD3	1:A:415:ILE:HG22	1.77	0.66
1:C:1187:VAL:HG12	1:D:1179:ASN:HD21	1.61	0.66
1:D:321:VAL:HG23	1:D:352:GLU:HG2	1.78	0.66
1:E:836:LEU:HB3	1:E:864:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LEU:HB3	1:A:864:LEU:HD11	1.78	0.66
1:A:321:VAL:HG23	1:A:352:GLU:HG2	1.78	0.66
1:E:334:ARG:HB2	1:E:434:PHE:HA	1.78	0.66
1:E:336:LYS:HD3	1:E:415:ILE:HG22	1.77	0.66
1:B:236:LEU:HD13	1:B:487:PHE:HB2	1.76	0.66
1:D:836:LEU:HB3	1:D:864:LEU:HD11	1.78	0.66
1:C:350:MET:HB2	1:C:359:ILE:HG13	1.78	0.65
1:C:2118:VAL:HG22	1:D:2242:ALA:HB3	1.78	0.65
1:A:2487:PHE:CZ	1:E:2364:GLU:HB3	2.31	0.65
1:B:600:LEU:HD11	1:B:628:THR:HG21	1.79	0.65
1:B:2102:ILE:HA	1:B:2261:GLN:NE2	2.12	0.65
1:A:2105:GLN:HB2	1:A:2261:GLN:HE22	1.61	0.65
1:D:743:LEU:HD22	1:D:750:ASN:HD21	1.62	0.65
1:D:750:ASN:HB2	1:D:754:THR:HG23	1.79	0.65
1:E:561:MET:HE3	1:E:567:ASN:HA	1.79	0.65
1:E:750:ASN:HB2	1:E:754:THR:HG23	1.79	0.65
1:D:2325:PHE:HB2	1:D:2351:MET:HE2	1.76	0.65
1:E:2105:GLN:HB2	1:E:2261:GLN:HE22	1.61	0.65
1:A:743:LEU:HD22	1:A:750:ASN:HD21	1.62	0.65
1:A:350:MET:HB2	1:A:359:ILE:HG13	1.78	0.65
1:B:321:VAL:HG23	1:B:352:GLU:HG2	1.78	0.65
1:B:336:LYS:HD3	1:B:415:ILE:HG22	1.77	0.65
1:B:750:ASN:HB2	1:B:754:THR:HG23	1.78	0.65
1:C:2121:GLU:OE1	1:D:2238:LYS:HG3	1.97	0.65
1:D:126:ALA:HA	1:D:129:LEU:HD23	1.79	0.65
1:D:2105:GLN:HB2	1:D:2261:GLN:HE22	1.61	0.65
1:B:350:MET:HB2	1:B:359:ILE:HG13	1.78	0.65
1:C:336:LYS:HD3	1:C:415:ILE:HG22	1.77	0.65
1:D:350:MET:HB2	1:D:359:ILE:HG13	1.78	0.65
1:D:561:MET:HE3	1:D:567:ASN:HA	1.79	0.65
1:D:2102:ILE:HA	1:D:2261:GLN:NE2	2.12	0.65
1:E:2102:ILE:HA	1:E:2261:GLN:NE2	2.12	0.65
1:A:2102:ILE:HA	1:A:2261:GLN:NE2	2.12	0.65
1:C:321:VAL:HG23	1:C:352:GLU:HG2	1.78	0.65
1:E:350:MET:HB2	1:E:359:ILE:HG13	1.78	0.65
1:A:2199:MET:HE2	1:E:2158:GLN:HE21	1.62	0.65
1:C:561:MET:HE3	1:C:567:ASN:HA	1.79	0.65
1:C:2102:ILE:HA	1:C:2261:GLN:NE2	2.12	0.65
1:D:2350:GLU:HG3	1:E:2302:LEU:HD11	1.79	0.65
1:A:334:ARG:HB2	1:A:434:PHE:HA	1.78	0.65
1:A:2199:MET:HE1	1:E:2158:GLN:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:LEU:HD11	1:C:628:THR:HG21	1.79	0.65
1:C:2105:GLN:HB2	1:C:2261:GLN:HE22	1.61	0.65
1:D:2536:ARG:HD3	1:E:2487:PHE:CZ	2.32	0.65
1:A:561:MET:HE3	1:A:567:ASN:HA	1.79	0.64
1:C:743:LEU:HD22	1:C:750:ASN:HD21	1.62	0.64
1:C:1116:ASN:HB2	1:D:1210:TRP:CD1	2.32	0.64
1:B:1813:PRO:HA	1:B:1832:TRP:HE1	1.63	0.64
1:C:1195:LEU:HD23	1:C:1214:ILE:HD12	1.80	0.64
1:C:1925:GLU:OE2	1:D:999:ARG:HG2	1.98	0.64
1:A:1813:PRO:HA	1:A:1832:TRP:HE1	1.63	0.64
1:A:2276:GLN:HB3	1:E:2033:MET:HE1	1.79	0.64
1:C:334:ARG:HB2	1:C:434:PHE:HA	1.78	0.64
1:D:600:LEU:HD11	1:D:628:THR:HG21	1.79	0.64
1:E:600:LEU:HD11	1:E:628:THR:HG21	1.79	0.64
1:A:750:ASN:HB2	1:A:754:THR:HG23	1.79	0.64
1:D:334:ARG:HB2	1:D:434:PHE:HA	1.78	0.64
1:D:1573:VAL:HG22	1:D:1588:LYS:HG2	1.80	0.64
1:D:1813:PRO:HA	1:D:1832:TRP:HE1	1.63	0.64
1:C:1813:PRO:HA	1:C:1832:TRP:HE1	1.63	0.64
1:E:743:LEU:HD22	1:E:750:ASN:HD21	1.62	0.64
1:E:1813:PRO:HA	1:E:1832:TRP:HE1	1.63	0.64
1:C:750:ASN:HB2	1:C:754:THR:HG23	1.79	0.64
1:E:373:LEU:HD23	1:E:380:SER:H	1.63	0.64
1:C:1573:VAL:HG22	1:C:1588:LYS:HG2	1.80	0.64
1:B:2105:GLN:HB2	1:B:2261:GLN:HE22	1.61	0.64
1:E:2051:TYR:HA	1:E:2495:ARG:HA	1.80	0.64
1:B:2212:LYS:HZ1	1:E:1065:GLN:HG3	1.63	0.63
1:B:126:ALA:HA	1:B:129:LEU:HD23	1.79	0.63
1:B:561:MET:HE3	1:B:567:ASN:HA	1.79	0.63
1:E:1195:LEU:HD23	1:E:1214:ILE:HD12	1.80	0.63
1:A:373:LEU:HD23	1:A:380:SER:H	1.63	0.63
1:A:600:LEU:HD11	1:A:628:THR:HG21	1.79	0.63
1:C:1385:GLY:HA3	1:C:1468:VAL:HB	1.80	0.63
1:B:334:ARG:HB2	1:B:434:PHE:HA	1.78	0.63
1:B:743:LEU:HD22	1:B:750:ASN:HD21	1.62	0.63
1:B:1937:GLN:HE21	1:C:290:LEU:HD21	1.63	0.63
1:D:2440:LYS:HD3	1:D:2538:THR:HG23	1.81	0.63
1:A:1573:VAL:HG22	1:A:1588:LYS:HG2	1.80	0.63
1:B:1385:GLY:HA3	1:B:1468:VAL:HB	1.80	0.63
1:A:126:ALA:HA	1:A:129:LEU:HD23	1.79	0.63
1:A:2051:TYR:HA	1:A:2495:ARG:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:GLN:HG3	1:D:2212:LYS:HZ1	1.63	0.63
1:C:126:ALA:HA	1:C:129:LEU:HD23	1.79	0.63
1:C:373:LEU:HD23	1:C:380:SER:H	1.63	0.63
1:D:1195:LEU:HD23	1:D:1214:ILE:HD12	1.80	0.63
1:D:2051:TYR:HA	1:D:2495:ARG:HA	1.80	0.63
1:A:1385:GLY:HA3	1:A:1468:VAL:HB	1.80	0.63
1:B:28:LEU:HD12	1:B:32:GLU:HB3	1.81	0.63
1:C:28:LEU:HD12	1:C:32:GLU:HB3	1.81	0.63
1:A:28:LEU:HD12	1:A:32:GLU:HB3	1.81	0.63
1:B:373:LEU:HD23	1:B:380:SER:H	1.63	0.63
1:B:1195:LEU:HD23	1:B:1214:ILE:HD12	1.80	0.63
1:B:2440:LYS:HD3	1:B:2538:THR:HG23	1.81	0.63
1:C:2051:TYR:HA	1:C:2495:ARG:HA	1.80	0.63
1:B:1573:VAL:HG22	1:B:1588:LYS:HG2	1.80	0.62
1:B:2051:TYR:HA	1:B:2495:ARG:HA	1.80	0.62
1:C:2440:LYS:HD3	1:C:2538:THR:HG23	1.81	0.62
1:D:373:LEU:HD23	1:D:380:SER:H	1.63	0.62
1:E:126:ALA:HA	1:E:129:LEU:HD23	1.79	0.62
1:B:230:ALA:HB2	1:B:894:VAL:HG13	1.81	0.62
1:C:230:ALA:HB2	1:C:894:VAL:HG13	1.81	0.62
1:D:1385:GLY:HA3	1:D:1468:VAL:HB	1.80	0.62
1:E:28:LEU:HD12	1:E:32:GLU:HB3	1.81	0.62
1:E:2440:LYS:HD3	1:E:2538:THR:HG23	1.81	0.62
1:A:1636:ARG:HD2	1:A:1643:THR:HG22	1.81	0.62
1:E:1636:ARG:HD2	1:E:1643:THR:HG22	1.81	0.62
1:A:2440:LYS:HD3	1:A:2538:THR:HG23	1.81	0.62
1:B:2187:ARG:HG2	1:B:2193:ARG:HH22	1.65	0.62
1:C:2179:PHE:HA	1:C:2183:CYS:HA	1.82	0.62
1:E:1573:VAL:HG22	1:E:1588:LYS:HG2	1.80	0.62
1:A:230:ALA:HB2	1:A:894:VAL:HG13	1.81	0.62
1:A:1195:LEU:HD23	1:A:1214:ILE:HD12	1.80	0.62
1:E:230:ALA:HB2	1:E:894:VAL:HG13	1.81	0.62
1:E:2187:ARG:HG2	1:E:2193:ARG:HH22	1.65	0.62
1:A:1106:LEU:HD21	1:A:1124:ASN:HB2	1.82	0.62
1:A:854:GLN:HA	1:A:857:VAL:HG22	1.82	0.62
1:D:1106:LEU:HD21	1:D:1124:ASN:HB2	1.82	0.62
1:A:2187:ARG:HG2	1:A:2193:ARG:HH22	1.65	0.62
1:C:1106:LEU:HD21	1:C:1124:ASN:HB2	1.82	0.62
1:D:28:LEU:HD12	1:D:32:GLU:HB3	1.81	0.62
1:D:230:ALA:HB2	1:D:894:VAL:HG13	1.81	0.62
1:D:2092:GLN:O	1:D:2095:MET:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:LEU:HD21	1:B:1124:ASN:HB2	1.82	0.62
1:B:1376:LYS:HG2	1:B:1415:ILE:HG13	1.82	0.62
1:C:2092:GLN:O	1:C:2095:MET:HG3	2.00	0.62
1:A:1376:LYS:HG2	1:A:1415:ILE:HG13	1.82	0.61
1:B:34:ARG:O	1:B:38:ASP:HB2	2.00	0.61
1:C:792:LEU:HA	1:C:867:TRP:HB3	1.82	0.61
1:C:2187:ARG:HG2	1:C:2193:ARG:HH22	1.65	0.61
1:E:1376:LYS:HG2	1:E:1415:ILE:HG13	1.82	0.61
1:B:2179:PHE:HA	1:B:2183:CYS:HA	1.82	0.61
1:C:122:LEU:HB3	1:C:993:ILE:HG21	1.82	0.61
1:A:34:ARG:O	1:A:38:ASP:HB2	2.00	0.61
1:A:2393:LEU:HD13	1:A:2526:GLU:HG2	1.82	0.61
1:B:1636:ARG:HD2	1:B:1643:THR:HG22	1.81	0.61
1:B:2393:LEU:HD13	1:B:2526:GLU:HG2	1.82	0.61
1:D:2179:PHE:HA	1:D:2183:CYS:HA	1.82	0.61
1:E:2393:LEU:HD13	1:E:2526:GLU:HG2	1.82	0.61
1:C:1214:ILE:HG12	1:C:1268:MET:HE3	1.83	0.61
1:D:792:LEU:HA	1:D:867:TRP:HB3	1.82	0.61
1:D:1214:ILE:HG12	1:D:1268:MET:HE3	1.83	0.61
1:E:792:LEU:HA	1:E:867:TRP:HB3	1.82	0.61
1:C:34:ARG:O	1:C:38:ASP:HB2	2.00	0.61
1:C:2393:LEU:HD13	1:C:2526:GLU:HG2	1.83	0.61
1:D:34:ARG:O	1:D:38:ASP:HB2	2.00	0.61
1:D:122:LEU:HB3	1:D:993:ILE:HG21	1.82	0.61
1:D:1636:ARG:HD2	1:D:1643:THR:HG22	1.81	0.61
1:A:1668:PRO:HA	1:A:1707:GLU:HG3	1.83	0.61
1:A:2192:LEU:HD11	1:E:2169:GLU:HG2	1.83	0.61
1:C:2458:ALA:HB3	1:C:2477:LEU:HB2	1.83	0.61
1:D:2187:ARG:HG2	1:D:2193:ARG:HH22	1.65	0.61
1:E:122:LEU:HB3	1:E:993:ILE:HG21	1.82	0.61
1:E:1385:GLY:HA3	1:E:1468:VAL:HB	1.80	0.61
1:E:2092:GLN:O	1:E:2095:MET:HG3	2.00	0.61
1:E:1106:LEU:HD21	1:E:1124:ASN:HB2	1.82	0.61
1:E:1668:PRO:HA	1:E:1707:GLU:HG3	1.83	0.61
1:A:2179:PHE:HA	1:A:2183:CYS:HA	1.82	0.60
1:B:1214:ILE:HG12	1:B:1268:MET:HE3	1.82	0.60
1:C:854:GLN:HA	1:C:857:VAL:HG22	1.82	0.60
1:C:2005:ARG:HG2	1:D:977:VAL:HA	1.83	0.60
1:D:854:GLN:HA	1:D:857:VAL:HG22	1.82	0.60
1:A:792:LEU:HA	1:A:867:TRP:HB3	1.82	0.60
1:B:2092:GLN:O	1:B:2095:MET:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1636:ARG:HD2	1:C:1643:THR:HG22	1.81	0.60
1:E:34:ARG:O	1:E:38:ASP:HB2	2.00	0.60
1:E:2179:PHE:HA	1:E:2183:CYS:HA	1.82	0.60
1:A:2458:ALA:HB3	1:A:2477:LEU:HB2	1.83	0.60
1:B:1634:VAL:HG22	1:C:1202:HIS:HE1	1.65	0.60
1:D:2393:LEU:HD13	1:D:2526:GLU:HG2	1.82	0.60
1:A:692:ALA:HB1	1:A:741:MET:HG3	1.84	0.60
1:A:1794:PRO:HB2	1:A:1856:ARG:HH22	1.67	0.60
1:B:792:LEU:HA	1:B:867:TRP:HB3	1.82	0.60
1:C:1343:GLN:HB2	1:C:1358:HIS:HB2	1.83	0.60
1:D:1343:GLN:HB2	1:D:1358:HIS:HB2	1.83	0.60
1:C:1794:PRO:HB2	1:C:1856:ARG:HH22	1.66	0.60
1:E:854:GLN:HA	1:E:857:VAL:HG22	1.82	0.60
1:C:1376:LYS:HG2	1:C:1415:ILE:HG13	1.82	0.60
1:D:1376:LYS:HG2	1:D:1415:ILE:HG13	1.82	0.60
1:A:2113:ASP:HA	1:A:2116:ILE:HG12	1.84	0.60
1:B:692:ALA:HB1	1:B:741:MET:HG3	1.84	0.60
1:D:1794:PRO:HB2	1:D:1856:ARG:HH22	1.66	0.60
1:B:854:GLN:HA	1:B:857:VAL:HG22	1.82	0.60
1:A:122:LEU:HB3	1:A:993:ILE:HG21	1.82	0.60
1:A:1214:ILE:HG12	1:A:1268:MET:HE3	1.83	0.60
1:B:2113:ASP:HA	1:B:2116:ILE:HG12	1.84	0.60
1:B:122:LEU:HB3	1:B:993:ILE:HG21	1.82	0.60
1:B:281:TRP:HA	1:B:284:LYS:HE3	1.84	0.60
1:B:1343:GLN:HB2	1:B:1358:HIS:HB2	1.83	0.59
1:C:1444:THR:HB	1:C:1453:ARG:HA	1.84	0.59
1:C:1668:PRO:HA	1:C:1707:GLU:HG3	1.83	0.59
1:A:281:TRP:HA	1:A:284:LYS:HE3	1.84	0.59
1:C:2148:ALA:HB2	1:D:2213:ILE:HD11	1.84	0.59
1:D:1668:PRO:HA	1:D:1707:GLU:HG3	1.83	0.59
1:E:1794:PRO:HB2	1:E:1856:ARG:HH22	1.66	0.59
1:B:1794:PRO:HB2	1:B:1856:ARG:HH22	1.66	0.59
1:B:2458:ALA:HB3	1:B:2477:LEU:HB2	1.83	0.59
1:E:2458:ALA:HB3	1:E:2477:LEU:HB2	1.83	0.59
1:A:1202:HIS:HB3	1:E:1078:LYS:HE2	1.84	0.59
1:B:1668:PRO:HA	1:B:1707:GLU:HG3	1.83	0.59
1:C:73:PRO:HB2	1:C:1931:PRO:HG3	1.85	0.59
1:C:281:TRP:HA	1:C:284:LYS:HE3	1.84	0.59
1:C:1490:ASN:H	1:C:1492:GLN:HE22	1.50	0.59
1:C:2100:GLN:O	1:C:2104:ILE:HG13	2.03	0.59
1:C:2113:ASP:HA	1:C:2116:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1444:THR:HB	1:D:1453:ARG:HA	1.84	0.59
1:E:1490:ASN:H	1:E:1492:GLN:HE22	1.50	0.59
1:B:1185:THR:HG23	1:C:1181:THR:HA	1.84	0.59
1:C:692:ALA:HB1	1:C:741:MET:HG3	1.84	0.59
1:D:1490:ASN:H	1:D:1492:GLN:HE22	1.50	0.59
1:D:2458:ALA:HB3	1:D:2477:LEU:HB2	1.83	0.59
1:E:692:ALA:HB1	1:E:741:MET:HG3	1.83	0.59
1:A:2100:GLN:O	1:A:2104:ILE:HG13	2.02	0.59
1:B:1717:ALA:HB3	1:B:1720:TYR:HB2	1.85	0.59
1:B:2100:GLN:O	1:B:2104:ILE:HG13	2.03	0.59
1:D:2100:GLN:O	1:D:2104:ILE:HG13	2.03	0.59
1:E:1214:ILE:HG12	1:E:1268:MET:HE3	1.83	0.59
1:A:2092:GLN:O	1:A:2095:MET:HG3	2.00	0.59
1:B:73:PRO:HB2	1:B:1931:PRO:HG3	1.85	0.59
1:D:2384:ASN:HB3	1:D:2387:GLU:HB3	1.85	0.59
1:A:73:PRO:HB2	1:A:1931:PRO:HG3	1.85	0.59
1:A:708:ILE:HG13	1:A:724:LEU:HD21	1.85	0.59
1:A:1490:ASN:H	1:A:1492:GLN:HE22	1.50	0.59
1:E:1741:TRP:HB3	1:E:1777:LYS:HB2	1.85	0.59
1:A:1343:GLN:HB2	1:A:1358:HIS:HB2	1.83	0.59
1:E:1343:GLN:HB2	1:E:1358:HIS:HB2	1.83	0.59
1:B:1419:ASN:HB3	1:B:1424:TYR:HB2	1.85	0.59
1:C:1217:GLN:HE21	1:C:1278:LYS:HE2	1.68	0.59
1:D:73:PRO:HB2	1:D:1931:PRO:HG3	1.85	0.59
1:E:2113:ASP:HA	1:E:2116:ILE:HG12	1.84	0.59
1:A:1925:GLU:HG2	1:B:1004:ILE:HD13	1.85	0.58
1:B:350:MET:HB2	1:B:359:ILE:HA	1.85	0.58
1:C:1717:ALA:HB3	1:C:1720:TYR:HB2	1.85	0.58
1:A:350:MET:HB2	1:A:359:ILE:HA	1.85	0.58
1:B:1217:GLN:HE21	1:B:1278:LYS:HE2	1.68	0.58
1:C:2064:VAL:HG11	1:C:2345:LEU:HG	1.85	0.58
1:A:1078:LYS:HE2	1:B:1202:HIS:HB3	1.85	0.58
1:B:2064:VAL:HG11	1:B:2345:LEU:HG	1.85	0.58
1:C:350:MET:HB2	1:C:359:ILE:HA	1.85	0.58
1:A:793:GLY:HA3	1:A:868:GLN:HG2	1.86	0.58
1:B:1687:ASN:HB3	1:B:1722:MET:SD	2.44	0.58
1:B:1741:TRP:HB3	1:B:1777:LYS:HB2	1.85	0.58
1:B:2384:ASN:HB3	1:B:2387:GLU:HB3	1.85	0.58
1:D:1419:ASN:HB3	1:D:1424:TYR:HB2	1.85	0.58
1:E:1717:ALA:HB3	1:E:1720:TYR:HB2	1.85	0.58
1:A:1444:THR:HB	1:A:1453:ARG:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:CE1	1:B:202:PRO:HG2	2.39	0.58
1:D:1217:GLN:HE21	1:D:1278:LYS:HE2	1.68	0.58
1:E:281:TRP:HA	1:E:284:LYS:HE3	1.84	0.58
1:E:614:LEU:HD12	1:E:617:LEU:HD11	1.86	0.58
1:E:1217:GLN:HE21	1:E:1278:LYS:HE2	1.68	0.58
1:A:614:LEU:HD12	1:A:617:LEU:HD11	1.86	0.58
1:C:614:LEU:HD12	1:C:617:LEU:HD11	1.86	0.58
1:C:1741:TRP:HB3	1:C:1777:LYS:HB2	1.85	0.58
1:C:2384:ASN:HB3	1:C:2387:GLU:HB3	1.85	0.58
1:D:692:ALA:HB1	1:D:741:MET:HG3	1.84	0.58
1:D:1687:ASN:HB3	1:D:1722:MET:SD	2.44	0.58
1:E:73:PRO:HB2	1:E:1931:PRO:HG3	1.85	0.58
1:D:614:LEU:HD12	1:D:617:LEU:HD11	1.86	0.58
1:D:1741:TRP:HB3	1:D:1777:LYS:HB2	1.84	0.58
1:D:2064:VAL:HG11	1:D:2345:LEU:HG	1.85	0.58
1:E:1444:THR:HB	1:E:1453:ARG:HA	1.85	0.58
1:A:1202:HIS:CE1	1:E:1634:VAL:HG22	2.39	0.58
1:A:2384:ASN:HB3	1:A:2387:GLU:HB3	1.85	0.58
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.86	0.58
1:B:1444:THR:HB	1:B:1453:ARG:HA	1.85	0.58
1:C:1255:TYR:HE2	1:C:1296:ILE:HG22	1.69	0.58
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.39	0.58
1:D:793:GLY:HA3	1:D:868:GLN:HG2	1.86	0.58
1:D:1717:ALA:HB3	1:D:1720:TYR:HB2	1.85	0.58
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.39	0.58
1:A:1255:TYR:HE2	1:A:1296:ILE:HG22	1.69	0.58
1:A:1717:ALA:HB3	1:A:1720:TYR:HB2	1.85	0.58
1:B:1117:LEU:HD11	1:D:2168:ALA:HA	1.85	0.58
1:B:1490:ASN:H	1:B:1492:GLN:HE22	1.50	0.58
1:D:281:TRP:HA	1:D:284:LYS:HE3	1.84	0.58
1:D:1150:VAL:HG12	1:D:1152:PRO:HD3	1.86	0.58
1:E:350:MET:HB2	1:E:359:ILE:HA	1.85	0.58
1:E:1150:VAL:HG12	1:E:1152:PRO:HD3	1.86	0.58
1:A:216:THR:HG22	1:A:494:HIS:HB3	1.86	0.57
1:A:1687:ASN:HB3	1:A:1722:MET:SD	2.44	0.57
1:C:708:ILE:HG13	1:C:724:LEU:HD21	1.85	0.57
1:C:793:GLY:HA3	1:C:868:GLN:HG2	1.86	0.57
1:E:793:GLY:HA3	1:E:868:GLN:HG2	1.86	0.57
1:E:1687:ASN:HB3	1:E:1722:MET:SD	2.44	0.57
1:E:2100:GLN:O	1:E:2104:ILE:HG13	2.03	0.57
1:A:1741:TRP:HB3	1:A:1777:LYS:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2353:LYS:HD2	1:B:2302:LEU:HD22	1.85	0.57
1:B:614:LEU:HD12	1:B:617:LEU:HD11	1.86	0.57
1:D:2113:ASP:HA	1:D:2116:ILE:HG12	1.84	0.57
1:E:708:ILE:HG13	1:E:724:LEU:HD21	1.85	0.57
1:B:793:GLY:HA3	1:B:868:GLN:HG2	1.86	0.57
1:E:2384:ASN:HB3	1:E:2387:GLU:HB3	1.85	0.57
1:A:1419:ASN:HB3	1:A:1424:TYR:HB2	1.85	0.57
1:C:200:HIS:CE1	1:C:202:PRO:HG2	2.39	0.57
1:E:1419:ASN:HB3	1:E:1424:TYR:HB2	1.85	0.57
1:A:242:ILE:HA	1:A:246:LEU:HD23	1.87	0.57
1:A:2158:GLN:O	1:B:2199:MET:HE1	2.04	0.57
1:B:216:THR:HG22	1:B:494:HIS:HB3	1.86	0.57
1:B:708:ILE:HG13	1:B:724:LEU:HD21	1.85	0.57
1:C:1687:ASN:HB3	1:C:1722:MET:SD	2.44	0.57
1:C:1841:GLY:HA3	1:D:1003:ARG:NH2	2.19	0.57
1:D:708:ILE:HG13	1:D:724:LEU:HD21	1.85	0.57
1:E:216:THR:HG22	1:E:494:HIS:HB3	1.86	0.57
1:C:1440:ARG:HG2	1:C:1458:PRO:HA	1.87	0.57
1:D:1906:ARG:HH22	1:D:2010:ILE:HG21	1.70	0.57
1:A:1217:GLN:HE21	1:A:1278:LYS:HE2	1.68	0.57
1:B:70:ARG:HH12	1:B:1883:MET:HE2	1.70	0.57
1:B:1440:ARG:HG2	1:B:1458:PRO:HA	1.87	0.57
1:C:242:ILE:HA	1:C:246:LEU:HD23	1.87	0.57
1:C:1065:GLN:HG3	1:E:2212:LYS:HZ1	1.70	0.57
1:D:70:ARG:HH12	1:D:1883:MET:HE2	1.70	0.57
1:A:2064:VAL:HG11	1:A:2345:LEU:HG	1.85	0.57
1:C:1419:ASN:HB3	1:C:1424:TYR:HB2	1.85	0.57
1:C:1906:ARG:HH22	1:C:2010:ILE:HG21	1.70	0.57
1:C:1412:GLY:HA3	1:C:1430:GLY:H	1.70	0.57
1:D:242:ILE:HA	1:D:246:LEU:HD23	1.87	0.57
1:D:350:MET:HB2	1:D:359:ILE:HA	1.85	0.57
1:D:1255:TYR:HE2	1:D:1296:ILE:HG22	1.69	0.57
1:E:334:ARG:HB3	1:E:434:PHE:HD1	1.69	0.57
1:E:1255:TYR:HE2	1:E:1296:ILE:HG22	1.69	0.57
1:C:334:ARG:HB3	1:C:434:PHE:HD1	1.69	0.57
1:E:1412:GLY:HA3	1:E:1430:GLY:H	1.70	0.57
1:E:2064:VAL:HG11	1:E:2345:LEU:HG	1.85	0.57
1:A:2170:GLY:HA3	1:A:2191:ALA:HA	1.87	0.56
1:B:1906:ARG:HH22	1:B:2010:ILE:HG21	1.70	0.56
1:C:1150:VAL:HG12	1:C:1152:PRO:HD3	1.86	0.56
1:D:348:ASP:HB2	1:D:359:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1412:GLY:HA3	1:D:1430:GLY:H	1.70	0.56
1:E:200:HIS:CE1	1:E:202:PRO:HG2	2.39	0.56
1:A:1440:ARG:HG2	1:A:1458:PRO:HA	1.87	0.56
1:B:1412:GLY:HA3	1:B:1430:GLY:H	1.70	0.56
1:D:2345:LEU:HD13	1:E:2066:GLN:HG2	1.88	0.56
1:A:1906:ARG:HH22	1:A:2010:ILE:HG21	1.70	0.56
1:B:242:ILE:HA	1:B:246:LEU:HD23	1.87	0.56
1:B:2033:MET:HE1	1:C:2276:GLN:HB3	1.87	0.56
1:C:70:ARG:HH12	1:C:1883:MET:HE2	1.70	0.56
1:C:216:THR:HG22	1:C:494:HIS:HB3	1.87	0.56
1:C:348:ASP:HB2	1:C:359:ILE:HG21	1.87	0.56
1:A:1150:VAL:HG12	1:A:1152:PRO:HD3	1.86	0.56
1:A:2518:THR:HB	1:A:2519:ASP:CG	2.31	0.56
1:B:348:ASP:HB2	1:B:359:ILE:HG21	1.87	0.56
1:D:334:ARG:HB3	1:D:434:PHE:HD1	1.69	0.56
1:D:1440:ARG:HG2	1:D:1458:PRO:HA	1.87	0.56
1:D:2170:GLY:HA3	1:D:2191:ALA:HA	1.87	0.56
1:E:2170:GLY:HA3	1:E:2191:ALA:HA	1.87	0.56
1:B:1255:TYR:HE2	1:B:1296:ILE:HG22	1.69	0.56
1:D:216:THR:HG22	1:D:494:HIS:HB3	1.86	0.56
1:E:348:ASP:HB2	1:E:359:ILE:HG21	1.87	0.56
1:E:1906:ARG:HH22	1:E:2010:ILE:HG21	1.70	0.56
1:A:334:ARG:HB3	1:A:434:PHE:HD1	1.69	0.56
1:E:1898:ILE:HD11	1:E:1923:THR:HG21	1.88	0.56
1:B:2169:GLU:HG2	1:C:2192:LEU:CD1	2.27	0.56
1:C:1416:THR:HG21	1:C:1443:LEU:HD21	1.88	0.56
1:A:70:ARG:HH12	1:A:1883:MET:HE2	1.70	0.56
1:B:2170:GLY:HA3	1:B:2191:ALA:HA	1.87	0.56
1:B:2212:LYS:NZ	1:E:1065:GLN:HG3	2.21	0.56
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.88	0.56
1:C:1021:TRP:HA	1:C:1024:ASN:HB2	1.88	0.56
1:E:1021:TRP:HA	1:E:1024:ASN:HB2	1.88	0.56
1:B:2518:THR:HB	1:B:2519:ASP:CG	2.31	0.56
1:C:1520:THR:HG22	1:C:1529:THR:HG23	1.88	0.56
1:D:2366:THR:O	1:E:2478:SER:HB2	2.06	0.56
1:E:242:ILE:HA	1:E:246:LEU:HD23	1.87	0.56
1:B:334:ARG:HB3	1:B:434:PHE:HD1	1.69	0.56
1:D:1898:ILE:HD11	1:D:1923:THR:HG21	1.88	0.56
1:D:2100:GLN:HB2	1:E:2260:TYR:HD2	1.70	0.56
1:C:2166:SER:HB2	1:C:2198:VAL:HG11	1.89	0.55
1:A:1412:GLY:HA3	1:A:1430:GLY:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.88	0.55
1:D:2518:THR:HB	1:D:2519:ASP:CG	2.31	0.55
1:A:348:ASP:HB2	1:A:359:ILE:HG21	1.88	0.55
1:B:1067:LYS:HZ2	1:D:2141:ILE:H	1.54	0.55
1:B:2141:ILE:H	1:E:1067:LYS:HZ2	1.54	0.55
1:C:2056:MET:HG3	1:C:2059:ARG:CZ	2.37	0.55
1:E:70:ARG:HH12	1:E:1883:MET:HE2	1.70	0.55
1:A:2166:SER:HB2	1:A:2198:VAL:HG11	1.89	0.55
1:B:362:ASN:HD21	1:B:364:LYS:HE3	1.72	0.55
1:B:1898:ILE:HD11	1:B:1923:THR:HG21	1.88	0.55
1:B:2166:SER:HB2	1:B:2198:VAL:HG11	1.89	0.55
1:E:1440:ARG:HG2	1:E:1458:PRO:HA	1.87	0.55
1:A:362:ASN:HD21	1:A:364:LYS:HE3	1.72	0.55
1:C:2170:GLY:HA3	1:C:2191:ALA:HA	1.87	0.55
1:D:119:LEU:HD13	1:D:986:LEU:HD22	1.89	0.55
1:D:2056:MET:HG3	1:D:2059:ARG:CZ	2.37	0.55
1:E:334:ARG:HB2	1:E:433:ILE:O	2.07	0.55
1:A:1520:THR:HG22	1:A:1529:THR:HG23	1.88	0.55
1:A:1639:THR:HG22	1:A:1640:GLY:H	1.72	0.55
1:B:28:LEU:HD21	1:B:33:LEU:HD12	1.89	0.55
1:B:200:HIS:HB3	1:B:203:TYR:HB3	1.88	0.55
1:C:848:ASP:CG	1:D:569:GLY:HA3	2.31	0.55
1:A:2056:MET:HG3	1:A:2059:ARG:CZ	2.37	0.55
1:B:1416:THR:HG21	1:B:1443:LEU:HD21	1.88	0.55
1:C:1887:ILE:HG22	1:C:1891:MET:HE2	1.89	0.55
1:C:1898:ILE:HD11	1:C:1923:THR:HG21	1.88	0.55
1:D:2166:SER:HB2	1:D:2198:VAL:HG11	1.89	0.55
1:E:1668:PRO:HG3	1:E:1783:LEU:HB2	1.89	0.55
1:A:1887:ILE:HG22	1:A:1891:MET:HE2	1.89	0.55
1:E:119:LEU:HD13	1:E:986:LEU:HD22	1.89	0.55
1:E:2166:SER:HB2	1:E:2198:VAL:HG11	1.88	0.55
1:B:1639:THR:HG22	1:B:1640:GLY:H	1.72	0.55
1:B:1887:ILE:HG22	1:B:1891:MET:HE2	1.89	0.55
1:C:119:LEU:HD13	1:C:986:LEU:HD22	1.89	0.55
1:C:334:ARG:HB2	1:C:433:ILE:O	2.07	0.55
1:C:362:ASN:HD21	1:C:364:LYS:HE3	1.71	0.55
1:D:1021:TRP:HA	1:D:1024:ASN:HB2	1.88	0.55
1:D:1416:THR:HG21	1:D:1443:LEU:HD21	1.88	0.55
1:D:1668:PRO:HG3	1:D:1783:LEU:HB2	1.89	0.55
1:D:2169:GLU:HG2	1:E:2192:LEU:HD11	1.88	0.55
1:E:2518:THR:HB	1:E:2519:ASP:CG	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD21	1:A:33:LEU:HD12	1.89	0.55
1:A:119:LEU:HD13	1:A:986:LEU:HD22	1.89	0.55
1:C:2158:GLN:HG2	1:D:2199:MET:HE2	1.88	0.55
1:C:2518:THR:HB	1:C:2519:ASP:CG	2.31	0.55
1:E:1520:THR:HG22	1:E:1529:THR:HG23	1.88	0.55
1:E:1887:ILE:HG22	1:E:1891:MET:HE2	1.89	0.55
1:A:1668:PRO:HG3	1:A:1783:LEU:HB2	1.89	0.54
1:A:2059:ARG:HA	1:A:2062:ASN:ND2	2.23	0.54
1:B:1624:ARG:HB2	1:B:1657:LEU:HD21	1.89	0.54
1:C:2158:GLN:HE21	1:D:2199:MET:HE2	1.72	0.54
1:D:1887:ILE:HG22	1:D:1891:MET:HE2	1.89	0.54
1:E:362:ASN:HD21	1:E:364:LYS:HE3	1.71	0.54
1:A:1898:ILE:HD11	1:A:1923:THR:HG21	1.88	0.54
1:A:2181:LEU:HD13	1:E:2181:LEU:HD21	1.89	0.54
1:B:1668:PRO:HG3	1:B:1783:LEU:HB2	1.89	0.54
1:B:2050:LEU:HG	1:B:2496:TYR:H	1.73	0.54
1:B:2059:ARG:HA	1:B:2062:ASN:ND2	2.23	0.54
1:B:2256:MET:O	1:B:2259:GLU:HG3	2.08	0.54
1:D:1324:MET:HE3	1:D:1574:PHE:CE2	2.43	0.54
1:D:2050:LEU:HG	1:D:2496:TYR:H	1.73	0.54
1:A:334:ARG:HB2	1:A:433:ILE:O	2.07	0.54
1:A:2050:LEU:HG	1:A:2496:TYR:H	1.73	0.54
1:B:119:LEU:HD13	1:B:986:LEU:HD22	1.89	0.54
1:B:697:ARG:HG2	1:B:737:ILE:HD12	1.90	0.54
1:B:2331:TRP:CD2	1:B:2337:GLY:HA3	2.43	0.54
1:C:1324:MET:HE3	1:C:1574:PHE:CE2	2.43	0.54
1:C:2059:ARG:HA	1:C:2062:ASN:ND2	2.23	0.54
1:C:2339:MET:HE3	1:D:2288:MET:SD	2.47	0.54
1:A:1416:THR:HG21	1:A:1443:LEU:HD21	1.88	0.54
1:A:1624:ARG:HB2	1:A:1657:LEU:HD21	1.89	0.54
1:B:886:MET:HE3	1:B:887:PRO:HD2	1.90	0.54
1:C:1668:PRO:HG3	1:C:1783:LEU:HB2	1.89	0.54
1:C:2050:LEU:HG	1:C:2496:TYR:H	1.73	0.54
1:C:2331:TRP:CD2	1:C:2337:GLY:HA3	2.43	0.54
1:D:697:ARG:HG2	1:D:737:ILE:HD12	1.90	0.54
1:D:1520:THR:HG22	1:D:1529:THR:HG23	1.88	0.54
1:D:1634:VAL:HG22	1:E:1202:HIS:CE1	2.42	0.54
1:E:350:MET:HG3	1:E:352:GLU:H	1.73	0.54
1:E:2059:ARG:HA	1:E:2062:ASN:ND2	2.22	0.54
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.88	0.54
1:B:2056:MET:HG3	1:B:2059:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1416:THR:HG21	1:E:1443:LEU:HD21	1.88	0.54
1:E:2050:LEU:HG	1:E:2496:TYR:H	1.73	0.54
1:E:2056:MET:HG3	1:E:2059:ARG:CZ	2.37	0.54
1:A:2239:GLN:HE22	1:E:2122:SER:HA	1.72	0.54
1:D:362:ASN:HD21	1:D:364:LYS:HE3	1.72	0.54
1:D:2123:ARG:NH1	1:D:2237:VAL:HG13	2.23	0.54
1:D:2331:TRP:CD2	1:D:2337:GLY:HA3	2.43	0.54
1:E:288:LEU:HG	1:E:452:ILE:HD11	1.90	0.54
1:E:1324:MET:HE3	1:E:1574:PHE:CE2	2.43	0.54
1:A:350:MET:HG3	1:A:352:GLU:H	1.73	0.54
1:B:350:MET:HG3	1:B:352:GLU:H	1.73	0.54
1:B:1021:TRP:HA	1:B:1024:ASN:HB2	1.88	0.54
1:C:28:LEU:HD21	1:C:33:LEU:HD12	1.89	0.54
1:D:350:MET:HG3	1:D:352:GLU:H	1.73	0.54
1:D:2256:MET:O	1:D:2259:GLU:HG3	2.08	0.54
1:E:200:HIS:HB3	1:E:203:TYR:HB3	1.88	0.54
1:E:1639:THR:HG22	1:E:1640:GLY:H	1.72	0.54
1:A:1021:TRP:HA	1:A:1024:ASN:HB2	1.88	0.54
1:B:1238:PHE:HB3	1:B:1243:THR:HG22	1.90	0.54
1:B:1520:THR:HG22	1:B:1529:THR:HG23	1.88	0.54
1:C:370:GLY:H	1:C:386:LEU:HD22	1.73	0.54
1:C:886:MET:HE3	1:C:887:PRO:HD2	1.90	0.54
1:E:370:GLY:H	1:E:386:LEU:HD22	1.73	0.54
1:A:288:LEU:HG	1:A:452:ILE:HD11	1.90	0.54
1:A:886:MET:HE3	1:A:887:PRO:HD2	1.90	0.54
1:A:1324:MET:HE3	1:A:1574:PHE:CE2	2.43	0.54
1:A:2331:TRP:CD2	1:A:2337:GLY:HA3	2.43	0.54
1:B:334:ARG:HB2	1:B:433:ILE:O	2.07	0.54
1:B:714:LEU:HD21	1:B:768:SER:HB2	1.90	0.54
1:B:2123:ARG:NH1	1:B:2237:VAL:HG13	2.23	0.54
1:C:288:LEU:HG	1:C:452:ILE:HD11	1.90	0.54
1:C:2256:MET:O	1:C:2259:GLU:HG3	2.08	0.54
1:D:1624:ARG:HB2	1:D:1657:LEU:HD21	1.89	0.54
1:B:2158:GLN:HE21	1:C:2199:MET:HE2	1.73	0.54
1:D:1639:THR:HG22	1:D:1640:GLY:H	1.72	0.54
1:C:1238:PHE:HB3	1:C:1243:THR:HG22	1.90	0.53
1:C:1639:THR:HG22	1:C:1640:GLY:H	1.72	0.53
1:D:1197:LEU:O	1:D:1209:PRO:HA	2.09	0.53
1:E:1624:ARG:HB2	1:E:1657:LEU:HD21	1.89	0.53
1:A:1238:PHE:HB3	1:A:1243:THR:HG22	1.90	0.53
1:A:1494:PHE:CD2	1:A:1496:ILE:HG12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ARG:HG2	1:C:737:ILE:HD12	1.90	0.53
1:D:14:THR:O	1:D:15:ARG:HD3	2.09	0.53
1:E:2256:MET:O	1:E:2259:GLU:HG3	2.08	0.53
1:E:2521:GLN:HE21	1:E:2524:LEU:HD23	1.73	0.53
1:A:2212:LYS:NZ	1:D:1065:GLN:HG3	2.23	0.53
1:A:2521:GLN:HE21	1:A:2524:LEU:HD23	1.73	0.53
1:B:1197:LEU:O	1:B:1209:PRO:HA	2.09	0.53
1:D:2059:ARG:HA	1:D:2062:ASN:ND2	2.23	0.53
1:E:1494:PHE:CD2	1:E:1496:ILE:HG12	2.43	0.53
1:B:288:LEU:HG	1:B:452:ILE:HD11	1.90	0.53
1:B:1324:MET:HE3	1:B:1574:PHE:CE2	2.43	0.53
1:C:2116:ILE:HG22	1:C:2247:LEU:HB3	1.91	0.53
1:D:2521:GLN:HE21	1:D:2524:LEU:HD23	1.73	0.53
1:A:535:LYS:HD3	1:A:536:ILE:H	1.72	0.53
1:A:697:ARG:HG2	1:A:737:ILE:HD12	1.90	0.53
1:A:738:ALA:HA	1:A:741:MET:SD	2.48	0.53
1:B:2462:TYR:HB2	1:B:2499:PHE:HE1	1.74	0.53
1:C:738:ALA:HA	1:C:741:MET:SD	2.48	0.53
1:C:1197:LEU:O	1:C:1209:PRO:HA	2.09	0.53
1:C:2521:GLN:HE21	1:C:2524:LEU:HD23	1.73	0.53
1:D:334:ARG:HB2	1:D:433:ILE:O	2.07	0.53
1:D:410:LYS:HA	1:D:410:LYS:HE3	1.91	0.53
1:E:1197:LEU:O	1:E:1209:PRO:HA	2.09	0.53
1:E:2331:TRP:CD2	1:E:2337:GLY:HA3	2.43	0.53
1:A:714:LEU:HD21	1:A:768:SER:HB2	1.90	0.53
1:C:1494:PHE:CD2	1:C:1496:ILE:HG12	2.43	0.53
1:D:817:ILE:HA	1:D:820:LEU:HG	1.91	0.53
1:E:14:THR:O	1:E:15:ARG:HD3	2.09	0.53
1:E:535:LYS:HD3	1:E:536:ILE:H	1.72	0.53
1:A:2462:TYR:HB2	1:A:2499:PHE:HE1	1.74	0.53
1:B:535:LYS:HD3	1:B:536:ILE:H	1.72	0.53
1:B:2116:ILE:HG22	1:B:2247:LEU:HB3	1.91	0.53
1:B:2346:LEU:HD22	1:C:2295:ILE:HG23	1.89	0.53
1:C:535:LYS:HD3	1:C:536:ILE:H	1.72	0.53
1:C:1624:ARG:HB2	1:C:1657:LEU:HD21	1.89	0.53
1:C:2118:VAL:HG22	1:D:2242:ALA:CB	2.38	0.53
1:C:2123:ARG:NH1	1:C:2237:VAL:HG13	2.23	0.53
1:D:1457:PHE:HZ	1:D:1471:VAL:HG22	1.74	0.53
1:D:535:LYS:HD3	1:D:536:ILE:H	1.72	0.53
1:D:886:MET:HE3	1:D:887:PRO:HD2	1.90	0.53
1:E:697:ARG:HG2	1:E:737:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD21	1:E:1937:GLN:HE21	1.73	0.53
1:A:1197:LEU:O	1:A:1209:PRO:HA	2.09	0.53
1:A:1457:PHE:HZ	1:A:1471:VAL:HG22	1.74	0.53
1:B:1151:ASN:HD21	1:D:2191:ALA:HB3	1.74	0.53
1:C:335:VAL:O	1:C:432:GLY:HA3	2.09	0.53
1:D:28:LEU:HD21	1:D:33:LEU:HD12	1.89	0.53
1:E:28:LEU:HD21	1:E:33:LEU:HD12	1.89	0.53
1:E:714:LEU:HD21	1:E:768:SER:HB2	1.90	0.53
1:A:370:GLY:H	1:A:386:LEU:HD22	1.73	0.53
1:A:1917:LYS:HG2	1:A:2004:LEU:HD13	1.91	0.53
1:A:2375:TYR:HD2	1:A:2385:LEU:HD13	1.74	0.53
1:C:850:SER:HB3	1:D:548:PRO:HB2	1.91	0.53
1:D:2116:ILE:HG22	1:D:2247:LEU:HB3	1.91	0.53
1:E:2462:TYR:HB2	1:E:2499:PHE:HE1	1.74	0.53
1:B:335:VAL:O	1:B:432:GLY:HA3	2.09	0.52
1:B:370:GLY:H	1:B:386:LEU:HD22	1.73	0.52
1:B:738:ALA:HA	1:B:741:MET:SD	2.48	0.52
1:B:1457:PHE:HZ	1:B:1471:VAL:HG22	1.74	0.52
1:B:2375:TYR:HD2	1:B:2385:LEU:HD13	1.74	0.52
1:C:350:MET:HE3	1:C:351:TYR:H	1.74	0.52
1:C:1041:GLU:HG3	1:C:1891:MET:HE1	1.92	0.52
1:C:1632:GLN:O	1:C:1636:ARG:HG2	2.10	0.52
1:D:288:LEU:HG	1:D:452:ILE:HD11	1.90	0.52
1:D:2284:LEU:O	1:D:2288:MET:HG2	2.10	0.52
1:E:335:VAL:O	1:E:432:GLY:HA3	2.09	0.52
1:E:1917:LYS:HG2	1:E:2004:LEU:HD13	1.91	0.52
1:A:2284:LEU:O	1:A:2288:MET:HG2	2.10	0.52
1:B:14:THR:O	1:B:15:ARG:HD3	2.09	0.52
1:D:738:ALA:HA	1:D:741:MET:SD	2.48	0.52
1:E:334:ARG:CB	1:E:434:PHE:HA	2.39	0.52
1:E:817:ILE:HA	1:E:820:LEU:HG	1.91	0.52
1:E:886:MET:HE3	1:E:887:PRO:HD2	1.90	0.52
1:E:2284:LEU:O	1:E:2288:MET:HG2	2.10	0.52
1:A:1925:GLU:OE2	1:B:999:ARG:HG2	2.10	0.52
1:A:2256:MET:O	1:A:2259:GLU:HG3	2.08	0.52
1:B:2284:LEU:O	1:B:2288:MET:HG2	2.10	0.52
1:C:313:ASP:HA	1:C:331:LYS:HE2	1.91	0.52
1:C:350:MET:HG3	1:C:352:GLU:H	1.73	0.52
1:C:2284:LEU:O	1:C:2288:MET:HG2	2.10	0.52
1:D:370:GLY:H	1:D:386:LEU:HD22	1.73	0.52
1:D:1238:PHE:HB3	1:D:1243:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:LYS:HA	1:E:410:LYS:HE3	1.91	0.52
1:E:1238:PHE:HB3	1:E:1243:THR:HG22	1.90	0.52
1:A:2116:ILE:HG22	1:A:2247:LEU:HB3	1.91	0.52
1:B:410:LYS:HE3	1:B:410:LYS:HA	1.91	0.52
1:B:817:ILE:HA	1:B:820:LEU:HG	1.91	0.52
1:B:1494:PHE:CD2	1:B:1496:ILE:HG12	2.43	0.52
1:C:14:THR:O	1:C:15:ARG:HD3	2.08	0.52
1:C:1457:PHE:HZ	1:C:1471:VAL:HG22	1.74	0.52
1:D:335:VAL:O	1:D:432:GLY:HA3	2.09	0.52
1:E:738:ALA:HA	1:E:741:MET:SD	2.48	0.52
1:A:1632:GLN:O	1:A:1636:ARG:HG2	2.10	0.52
1:B:1041:GLU:HG3	1:B:1891:MET:HE1	1.92	0.52
1:B:1917:LYS:HG2	1:B:2004:LEU:HD13	1.91	0.52
1:C:192:ARG:HG2	1:C:266:ASN:HA	1.92	0.52
1:C:714:LEU:HD21	1:C:768:SER:HB2	1.90	0.52
1:C:2133:TYR:CE1	1:D:2228:ILE:HG21	2.45	0.52
1:C:2155:ALA:HB1	1:D:2203:ALA:HB1	1.89	0.52
1:D:714:LEU:HD21	1:D:768:SER:HB2	1.90	0.52
1:D:2462:TYR:HB2	1:D:2499:PHE:HE1	1.74	0.52
1:A:817:ILE:HA	1:A:820:LEU:HG	1.91	0.52
1:C:972:LEU:HA	1:C:995:LEU:HD23	1.92	0.52
1:D:192:ARG:HG2	1:D:266:ASN:HA	1.92	0.52
1:A:14:THR:O	1:A:15:ARG:HD3	2.08	0.52
1:A:410:LYS:HA	1:A:410:LYS:HE3	1.90	0.52
1:B:2521:GLN:HE21	1:B:2524:LEU:HD23	1.73	0.52
1:C:410:LYS:HA	1:C:410:LYS:HE3	1.91	0.52
1:D:1041:GLU:HG3	1:D:1891:MET:HE1	1.92	0.52
1:E:2375:TYR:HD2	1:E:2385:LEU:HD13	1.74	0.52
1:B:350:MET:HE3	1:B:351:TYR:H	1.74	0.52
1:D:21:THR:HG23	1:D:24:ASP:H	1.75	0.52
1:D:1632:GLN:O	1:D:1636:ARG:HG2	2.10	0.52
1:E:2116:ILE:HG22	1:E:2247:LEU:HB3	1.91	0.52
1:A:2123:ARG:NH1	1:A:2237:VAL:HG13	2.23	0.52
1:C:2238:LYS:HA	1:C:2241:ASP:HB2	1.92	0.52
1:D:1494:PHE:CD2	1:D:1496:ILE:HG12	2.43	0.52
1:A:1637:ALA:HA	1:A:1644:ILE:HD11	1.92	0.52
1:B:1521:VAL:HG11	1:B:1556:ILE:HD13	1.92	0.52
1:B:2238:LYS:HA	1:B:2241:ASP:HB2	1.92	0.52
1:C:545:SER:HA	1:C:586:THR:HA	1.92	0.52
1:C:817:ILE:HA	1:C:820:LEU:HG	1.91	0.52
1:C:2462:TYR:HB2	1:C:2499:PHE:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ARG:CB	1:D:434:PHE:HA	2.39	0.52
1:D:350:MET:HE3	1:D:351:TYR:H	1.74	0.52
1:D:545:SER:HA	1:D:586:THR:HA	1.92	0.52
1:E:1599:ASN:O	1:E:1603:ILE:HG12	2.10	0.52
1:B:545:SER:HA	1:B:586:THR:HA	1.93	0.51
1:B:1599:ASN:O	1:B:1603:ILE:HG12	2.10	0.51
1:B:2058:GLU:HA	1:B:2061:ARG:HE	1.75	0.51
1:E:313:ASP:HA	1:E:331:LYS:HE2	1.91	0.51
1:E:1455:PHE:HE1	1:E:1478:ASP:HB3	1.75	0.51
1:A:335:VAL:O	1:A:432:GLY:HA3	2.09	0.51
1:B:21:THR:HG23	1:B:24:ASP:H	1.75	0.51
1:B:233:ALA:HB1	1:B:898:TYR:HB3	1.93	0.51
1:B:334:ARG:CB	1:B:434:PHE:HA	2.39	0.51
1:D:434:PHE:CZ	1:D:436:PHE:HB2	2.45	0.51
1:D:2111:GLU:OE1	1:E:2250:ARG:HG3	2.10	0.51
1:E:545:SER:HB2	1:E:586:THR:HG22	1.93	0.51
1:E:1457:PHE:HZ	1:E:1471:VAL:HG22	1.74	0.51
1:A:21:THR:HG23	1:A:24:ASP:H	1.75	0.51
1:A:545:SER:HA	1:A:586:THR:HA	1.92	0.51
1:A:2058:GLU:HA	1:A:2061:ARG:HE	1.75	0.51
1:B:313:ASP:HA	1:B:331:LYS:HE2	1.91	0.51
1:B:663:LEU:HD21	1:B:769:LEU:HG	1.92	0.51
1:C:334:ARG:CB	1:C:434:PHE:HA	2.39	0.51
1:C:663:LEU:HD21	1:C:769:LEU:HG	1.92	0.51
1:A:972:LEU:HA	1:A:995:LEU:HD23	1.92	0.51
1:A:1647:MET:HG3	1:A:1851:TRP:CE2	2.46	0.51
1:C:1521:VAL:HG11	1:C:1556:ILE:HD13	1.92	0.51
1:D:663:LEU:HD21	1:D:769:LEU:HG	1.92	0.51
1:D:1599:ASN:O	1:D:1603:ILE:HG12	2.10	0.51
1:D:1978:LEU:HD12	1:D:1978:LEU:O	2.11	0.51
1:E:350:MET:HE3	1:E:351:TYR:H	1.74	0.51
1:E:1632:GLN:O	1:E:1636:ARG:HG2	2.10	0.51
1:A:545:SER:HB2	1:A:586:THR:HG22	1.93	0.51
1:A:1041:GLU:HG3	1:A:1891:MET:HE1	1.92	0.51
1:B:986:LEU:O	1:B:990:ILE:HG12	2.11	0.51
1:B:1632:GLN:O	1:B:1636:ARG:HG2	2.10	0.51
1:C:2375:TYR:HD2	1:C:2385:LEU:HD13	1.74	0.51
1:D:1647:MET:HG3	1:D:1851:TRP:CE2	2.46	0.51
1:D:2058:GLU:HA	1:D:2061:ARG:HE	1.75	0.51
1:E:21:THR:HG23	1:E:24:ASP:H	1.75	0.51
1:E:1464:ILE:HG12	1:E:1466:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:SER:HB2	1:B:586:THR:HG22	1.93	0.51
1:C:434:PHE:CZ	1:C:436:PHE:HB2	2.45	0.51
1:C:2254:ALA:O	1:C:2258:VAL:HG23	2.11	0.51
1:E:1647:MET:HG3	1:E:1851:TRP:CE2	2.46	0.51
1:A:192:ARG:HG2	1:A:266:ASN:HA	1.92	0.51
1:A:233:ALA:HB1	1:A:898:TYR:HB3	1.93	0.51
1:A:334:ARG:CB	1:A:434:PHE:HA	2.39	0.51
1:A:1521:VAL:HG11	1:A:1556:ILE:HD13	1.92	0.51
1:A:1599:ASN:O	1:A:1603:ILE:HG12	2.10	0.51
1:A:2168:ALA:HA	1:D:1117:LEU:HD11	1.92	0.51
1:A:2503:SER:HB3	1:A:2506:ASP:HB2	1.93	0.51
1:B:663:LEU:HD11	1:B:769:LEU:HD23	1.93	0.51
1:B:1067:LYS:HD2	1:D:2146:GLN:HE21	1.76	0.51
1:B:1647:MET:HG3	1:B:1851:TRP:CE2	2.46	0.51
1:C:233:ALA:HB1	1:C:898:TYR:HB3	1.93	0.51
1:C:986:LEU:O	1:C:990:ILE:HG12	2.11	0.51
1:D:336:LYS:HB2	1:D:431:GLY:N	2.26	0.51
1:D:545:SER:HB2	1:D:586:THR:HG22	1.93	0.51
1:D:1455:PHE:HE1	1:D:1478:ASP:HB3	1.75	0.51
1:E:545:SER:HA	1:E:586:THR:HA	1.92	0.51
1:E:2238:LYS:HA	1:E:2241:ASP:HB2	1.92	0.51
1:A:350:MET:HE3	1:A:351:TYR:H	1.74	0.51
1:A:709:ALA:HA	1:A:714:LEU:HB2	1.93	0.51
1:A:2105:GLN:HB2	1:A:2261:GLN:NE2	2.26	0.51
1:B:439:TYR:HD1	1:B:443:ILE:HD12	1.75	0.51
1:B:1408:TYR:HB2	1:B:1433:MET:HE1	1.93	0.51
1:B:1637:ALA:HA	1:B:1644:ILE:HD11	1.92	0.51
1:C:1647:MET:HG3	1:C:1851:TRP:CE2	2.46	0.51
1:C:1917:LYS:HG2	1:C:2004:LEU:HD13	1.91	0.51
1:D:1464:ILE:HG12	1:D:1466:ASN:H	1.75	0.51
1:E:336:LYS:HB2	1:E:431:GLY:N	2.26	0.51
1:E:1408:TYR:HB2	1:E:1433:MET:HE1	1.93	0.51
1:A:313:ASP:HA	1:A:331:LYS:HE2	1.91	0.51
1:B:546:ILE:HA	1:B:557:ARG:HD2	1.93	0.51
1:C:21:THR:HG23	1:C:24:ASP:H	1.75	0.51
1:C:546:ILE:HA	1:C:557:ARG:HD2	1.93	0.51
1:C:1637:ALA:HA	1:C:1644:ILE:HD11	1.92	0.51
1:C:1978:LEU:HD12	1:C:1978:LEU:O	2.11	0.51
1:D:546:ILE:HA	1:D:557:ARG:HD2	1.93	0.51
1:E:663:LEU:HD11	1:E:769:LEU:HD23	1.93	0.51
1:E:1041:GLU:HG3	1:E:1891:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1336:MET:HE1	1:E:1364:VAL:HG22	1.93	0.51
1:E:1637:ALA:HA	1:E:1644:ILE:HD11	1.92	0.51
1:B:336:LYS:HB2	1:B:431:GLY:N	2.26	0.51
1:C:336:LYS:HB2	1:C:431:GLY:N	2.26	0.51
1:C:1464:ILE:HG12	1:C:1466:ASN:H	1.75	0.51
1:D:198:PRO:HG3	1:D:245:GLU:HB3	1.93	0.51
1:D:439:TYR:HD1	1:D:443:ILE:HD12	1.75	0.51
1:D:986:LEU:O	1:D:990:ILE:HG12	2.11	0.51
1:D:2238:LYS:HA	1:D:2241:ASP:HB2	1.92	0.51
1:D:2254:ALA:O	1:D:2258:VAL:HG23	2.11	0.51
1:E:2058:GLU:HA	1:E:2061:ARG:HE	1.75	0.51
1:E:2503:SER:HB3	1:E:2506:ASP:HB2	1.93	0.51
1:A:434:PHE:CZ	1:A:436:PHE:HB2	2.45	0.50
1:B:2105:GLN:HB2	1:B:2261:GLN:NE2	2.26	0.50
1:C:2058:GLU:HA	1:C:2061:ARG:HE	1.75	0.50
1:C:2342:GLU:HG2	1:D:2295:ILE:HD13	1.92	0.50
1:C:2503:SER:HB3	1:C:2506:ASP:HB2	1.93	0.50
1:D:1917:LYS:HG2	1:D:2004:LEU:HD13	1.91	0.50
1:D:2375:TYR:HD2	1:D:2385:LEU:HD13	1.74	0.50
1:E:439:TYR:HD1	1:E:443:ILE:HD12	1.75	0.50
1:E:663:LEU:HD21	1:E:769:LEU:HG	1.92	0.50
1:E:2254:ALA:O	1:E:2258:VAL:HG23	2.11	0.50
1:A:546:ILE:HA	1:A:557:ARG:HD2	1.93	0.50
1:A:986:LEU:O	1:A:990:ILE:HG12	2.11	0.50
1:B:192:ARG:HG2	1:B:266:ASN:HA	1.92	0.50
1:B:709:ALA:HA	1:B:714:LEU:HB2	1.93	0.50
1:B:972:LEU:HA	1:B:995:LEU:HD23	1.92	0.50
1:A:336:LYS:HB2	1:A:431:GLY:N	2.26	0.50
1:B:1067:LYS:HD2	1:D:2146:GLN:NE2	2.26	0.50
1:B:1455:PHE:HE1	1:B:1478:ASP:HB3	1.75	0.50
1:B:1464:ILE:HG12	1:B:1466:ASN:H	1.75	0.50
1:C:1455:PHE:HE1	1:C:1478:ASP:HB3	1.75	0.50
1:D:313:ASP:HA	1:D:331:LYS:HE2	1.91	0.50
1:D:1060:LEU:HG	1:E:2147:ARG:NH1	2.26	0.50
1:B:434:PHE:CZ	1:B:436:PHE:HB2	2.46	0.50
1:B:2254:ALA:O	1:B:2258:VAL:HG23	2.11	0.50
1:D:1521:VAL:HG11	1:D:1556:ILE:HD13	1.92	0.50
1:E:198:PRO:HG3	1:E:245:GLU:HB3	1.93	0.50
1:E:233:ALA:HB1	1:E:898:TYR:HB3	1.93	0.50
1:E:546:ILE:HA	1:E:557:ARG:HD2	1.93	0.50
1:E:972:LEU:HA	1:E:995:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:986:LEU:O	1:E:990:ILE:HG12	2.11	0.50
1:A:663:LEU:HD11	1:A:769:LEU:HD23	1.93	0.50
1:A:663:LEU:HD21	1:A:769:LEU:HG	1.92	0.50
1:A:1978:LEU:HD12	1:A:1978:LEU:O	2.11	0.50
1:C:545:SER:HB2	1:C:586:THR:HG22	1.93	0.50
1:C:1336:MET:HE1	1:C:1364:VAL:HG22	1.93	0.50
1:C:1599:ASN:O	1:C:1603:ILE:HG12	2.10	0.50
1:C:2169:GLU:CD	1:D:2193:ARG:HD3	2.36	0.50
1:D:663:LEU:HD11	1:D:769:LEU:HD23	1.93	0.50
1:D:709:ALA:HA	1:D:714:LEU:HB2	1.93	0.50
1:D:1637:ALA:HA	1:D:1644:ILE:HD11	1.92	0.50
1:E:192:ARG:HG2	1:E:266:ASN:HA	1.92	0.50
1:E:1521:VAL:HG11	1:E:1556:ILE:HD13	1.92	0.50
1:E:2123:ARG:NH1	1:E:2237:VAL:HG13	2.23	0.50
1:A:2254:ALA:O	1:A:2258:VAL:HG23	2.11	0.50
1:B:1978:LEU:HD12	1:B:1978:LEU:O	2.11	0.50
1:C:923:GLU:O	1:C:926:LEU:HD22	2.12	0.50
1:D:26:GLN:HA	1:D:57:LYS:NZ	2.27	0.50
1:D:1336:MET:HE1	1:D:1364:VAL:HG22	1.93	0.50
1:E:434:PHE:CZ	1:E:436:PHE:HB2	2.46	0.50
1:E:2105:GLN:HB2	1:E:2261:GLN:NE2	2.26	0.50
1:A:198:PRO:HG3	1:A:245:GLU:HB3	1.93	0.50
1:A:1464:ILE:HG12	1:A:1466:ASN:H	1.75	0.50
1:A:2238:LYS:HA	1:A:2241:ASP:HB2	1.92	0.50
1:B:1157:ILE:HD12	1:B:1170:TRP:HB3	1.94	0.50
1:C:26:GLN:HA	1:C:57:LYS:NZ	2.27	0.50
1:C:1408:TYR:HB2	1:C:1433:MET:HE1	1.93	0.50
1:E:923:GLU:O	1:E:926:LEU:HD22	2.12	0.50
1:A:1408:TYR:HB2	1:A:1433:MET:HE1	1.93	0.50
1:B:923:GLU:O	1:B:926:LEU:HD22	2.12	0.50
1:C:413:VAL:HG12	1:C:433:ILE:HD12	1.94	0.50
1:D:972:LEU:HA	1:D:995:LEU:HD23	1.92	0.50
1:D:1408:TYR:HB2	1:D:1433:MET:HE1	1.93	0.50
1:E:413:VAL:HG12	1:E:433:ILE:HD12	1.94	0.50
1:E:1978:LEU:O	1:E:1978:LEU:HD12	2.11	0.50
1:A:439:TYR:HD1	1:A:443:ILE:HD12	1.75	0.49
1:B:26:GLN:HA	1:B:57:LYS:NZ	2.27	0.49
1:B:413:VAL:HG12	1:B:433:ILE:HD12	1.94	0.49
1:D:2158:GLN:O	1:E:2199:MET:HE1	2.11	0.49
1:A:26:GLN:HA	1:A:57:LYS:NZ	2.27	0.49
1:A:1447:GLU:HB2	1:A:1484:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:PHE:HE1	1:A:1478:ASP:HB3	1.75	0.49
1:B:198:PRO:HG3	1:B:245:GLU:HB3	1.93	0.49
1:C:198:PRO:HG3	1:C:245:GLU:HB3	1.93	0.49
1:C:439:TYR:HD1	1:C:443:ILE:HD12	1.75	0.49
1:D:413:VAL:HG12	1:D:433:ILE:HD12	1.94	0.49
1:B:2503:SER:HB3	1:B:2506:ASP:HB2	1.93	0.49
1:C:709:ALA:HA	1:C:714:LEU:HB2	1.93	0.49
1:C:1157:ILE:HD12	1:C:1170:TRP:HB3	1.94	0.49
1:D:233:ALA:HB1	1:D:898:TYR:HB3	1.93	0.49
1:A:1010:ALA:HB1	1:E:1848:ILE:HG13	1.95	0.49
1:B:126:ALA:HB2	1:B:997:ILE:HD11	1.94	0.49
1:B:1177:ALA:HB3	1:C:2179:PHE:CZ	2.48	0.49
1:C:1447:GLU:HB2	1:C:1484:TYR:CD2	2.47	0.49
1:D:2097:LEU:HD22	1:E:2260:TYR:CE2	2.47	0.49
1:A:1292:ASN:HB3	1:A:1600:PRO:HG3	1.95	0.49
1:B:1065:GLN:HG3	1:D:2212:LYS:NZ	2.25	0.49
1:B:1447:GLU:HB2	1:B:1484:TYR:CD2	2.47	0.49
1:C:663:LEU:HD11	1:C:769:LEU:HD23	1.93	0.49
1:C:2111:GLU:OE1	1:D:2250:ARG:HG3	2.11	0.49
1:D:2503:SER:HB3	1:D:2506:ASP:HB2	1.93	0.49
1:E:26:GLN:HA	1:E:57:LYS:NZ	2.27	0.49
1:A:2169:GLU:HG2	1:B:2192:LEU:HD11	1.94	0.49
1:B:1336:MET:HE1	1:B:1364:VAL:HG22	1.93	0.49
1:C:1647:MET:HE2	1:C:1647:MET:HA	1.95	0.49
1:D:923:GLU:O	1:D:926:LEU:HD22	2.12	0.49
1:E:709:ALA:HA	1:E:714:LEU:HB2	1.93	0.49
1:B:1647:MET:HE2	1:B:1647:MET:HA	1.95	0.49
1:C:1292:ASN:HB3	1:C:1600:PRO:HG3	1.95	0.49
1:A:126:ALA:HB2	1:A:997:ILE:HD11	1.94	0.49
1:A:291:SER:O	1:A:295:LYS:HG2	2.12	0.49
1:A:1647:MET:HE1	1:A:1856:ARG:N	2.28	0.49
1:C:2212:LYS:HZ2	1:C:2213:ILE:HG22	1.78	0.49
1:E:1157:ILE:HD12	1:E:1170:TRP:HB3	1.94	0.49
1:E:1447:GLU:HB2	1:E:1484:TYR:CD2	2.47	0.49
1:A:1157:ILE:HD12	1:A:1170:TRP:HB3	1.94	0.49
1:B:1292:ASN:HB3	1:B:1600:PRO:HG3	1.95	0.49
1:C:1634:VAL:HG12	1:D:1164:GLU:OE2	2.12	0.49
1:D:1292:ASN:HB3	1:D:1600:PRO:HG3	1.95	0.49
1:D:1647:MET:HA	1:D:1647:MET:HE2	1.95	0.49
1:D:2105:GLN:HB2	1:D:2261:GLN:NE2	2.26	0.49
1:E:291:SER:O	1:E:295:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2446:LEU:HD22	1:E:2531:ILE:HD12	1.94	0.49
1:B:2446:LEU:HD22	1:B:2531:ILE:HD12	1.94	0.49
1:C:2169:GLU:HG3	1:D:2193:ARG:HB3	1.95	0.49
1:C:2446:LEU:HD22	1:C:2531:ILE:HD12	1.94	0.49
1:E:1647:MET:HE2	1:E:1647:MET:HA	1.95	0.49
1:E:2119:LEU:HB3	1:E:2244:LEU:HD13	1.95	0.49
1:E:2525:LEU:HA	1:E:2528:LEU:HB3	1.95	0.49
1:A:1336:MET:HE1	1:A:1364:VAL:HG22	1.93	0.48
1:B:266:ASN:HD22	1:B:446:LEU:HD22	1.78	0.48
1:B:2056:MET:HG3	1:B:2059:ARG:NH2	2.28	0.48
1:B:2140:ASP:HB3	1:E:1067:LYS:HZ1	1.78	0.48
1:E:1292:ASN:HB3	1:E:1600:PRO:HG3	1.95	0.48
1:A:923:GLU:O	1:A:926:LEU:HD22	2.12	0.48
1:A:1647:MET:HA	1:A:1647:MET:HE2	1.95	0.48
1:B:1647:MET:HE1	1:B:1856:ARG:N	2.28	0.48
1:C:126:ALA:HB2	1:C:997:ILE:HD11	1.94	0.48
1:C:337:THR:HB	1:C:430:GLY:HA2	1.95	0.48
1:C:2158:GLN:NE2	1:D:2199:MET:O	2.44	0.48
1:D:291:SER:O	1:D:295:LYS:HG2	2.12	0.48
1:D:1647:MET:HE1	1:D:1856:ARG:N	2.28	0.48
1:E:726:TRP:NE1	1:E:785:VAL:HG22	2.29	0.48
1:B:2119:LEU:HB3	1:B:2244:LEU:HD13	1.96	0.48
1:B:2518:THR:HB	1:B:2519:ASP:OD2	2.13	0.48
1:D:1622:ARG:HD2	1:D:1715:PRO:HB3	1.95	0.48
1:E:2426:PHE:HD2	1:E:2505:ASN:HD22	1.62	0.48
1:A:266:ASN:HD22	1:A:446:LEU:HD22	1.78	0.48
1:A:2056:MET:HG3	1:A:2059:ARG:NH2	2.28	0.48
1:A:2426:PHE:HD2	1:A:2505:ASN:HD22	1.61	0.48
1:A:2446:LEU:HD22	1:A:2531:ILE:HD12	1.94	0.48
1:C:2119:LEU:HB3	1:C:2244:LEU:HD13	1.95	0.48
1:C:2518:THR:HB	1:C:2519:ASP:OD2	2.14	0.48
1:D:1447:GLU:HB2	1:D:1484:TYR:CD2	2.47	0.48
1:B:291:SER:O	1:B:295:LYS:HG2	2.13	0.48
1:B:726:TRP:NE1	1:B:785:VAL:HG22	2.29	0.48
1:C:2056:MET:HG3	1:C:2059:ARG:NH2	2.28	0.48
1:C:2105:GLN:HB2	1:C:2261:GLN:NE2	2.26	0.48
1:D:2121:GLU:OE2	1:E:2239:GLN:OE1	2.31	0.48
1:E:337:THR:HB	1:E:430:GLY:HA2	1.95	0.48
1:E:1167:HIS:ND1	1:E:1199:PHE:HB3	2.28	0.48
1:E:1622:ARG:HD2	1:E:1715:PRO:HB3	1.95	0.48
1:A:337:THR:HB	1:A:430:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG12	1:A:433:ILE:HD12	1.94	0.48
1:B:206:ILE:HG23	1:B:922:MET:HE3	1.96	0.48
1:B:1848:ILE:HG23	1:C:1003:ARG:NH2	2.29	0.48
1:C:291:SER:O	1:C:295:LYS:HG2	2.13	0.48
1:C:842:ALA:HB2	1:C:852:VAL:HG21	1.96	0.48
1:C:2158:GLN:HG2	1:D:2199:MET:CE	2.44	0.48
1:D:1577:LYS:NZ	1:D:1581:GLY:HA2	2.29	0.48
1:D:2119:LEU:HB3	1:D:2244:LEU:HD13	1.95	0.48
1:E:409:TYR:CD2	1:E:410:LYS:HD2	2.49	0.48
1:E:1577:LYS:NZ	1:E:1581:GLY:HA2	2.29	0.48
1:A:2111:GLU:OE1	1:B:2250:ARG:HG3	2.13	0.48
1:A:2119:LEU:HB3	1:A:2244:LEU:HD13	1.96	0.48
1:B:409:TYR:CD2	1:B:410:LYS:HD2	2.49	0.48
1:D:126:ALA:HB2	1:D:997:ILE:HD11	1.94	0.48
1:D:266:ASN:HD22	1:D:446:LEU:HD22	1.78	0.48
1:D:409:TYR:CD2	1:D:410:LYS:HD2	2.49	0.48
1:D:2345:LEU:CD1	1:E:2066:GLN:HG2	2.44	0.48
1:E:1647:MET:HE1	1:E:1856:ARG:N	2.28	0.48
1:A:2518:THR:HB	1:A:2519:ASP:OD2	2.13	0.48
1:B:2107:ARG:O	1:B:2111:GLU:HG2	2.14	0.48
1:C:266:ASN:HD22	1:C:446:LEU:HD22	1.78	0.48
1:C:1577:LYS:NZ	1:C:1581:GLY:HA2	2.29	0.48
1:C:2152:LEU:CD2	1:D:2207:GLN:HG3	2.44	0.48
1:D:842:ALA:HB2	1:D:852:VAL:HG21	1.96	0.48
1:D:2107:ARG:O	1:D:2111:GLU:HG2	2.14	0.48
1:D:2242:ALA:O	1:D:2245:GLU:HG3	2.14	0.48
1:D:2446:LEU:HD22	1:D:2531:ILE:HD12	1.94	0.48
1:E:842:ALA:HB2	1:E:852:VAL:HG21	1.96	0.48
1:A:726:TRP:NE1	1:A:785:VAL:HG22	2.29	0.48
1:A:1167:HIS:ND1	1:A:1199:PHE:HB3	2.28	0.48
1:A:1937:GLN:HE21	1:B:290:LEU:HD11	1.78	0.48
1:A:2525:LEU:HA	1:A:2528:LEU:HB3	1.95	0.48
1:C:2121:GLU:OE2	1:D:2239:GLN:HA	2.13	0.48
1:C:2456:ILE:HG23	1:C:2524:LEU:HD21	1.96	0.48
1:D:1157:ILE:HD12	1:D:1170:TRP:HB3	1.94	0.48
1:D:1937:GLN:NE2	1:E:290:LEU:HD21	2.27	0.48
1:D:2056:MET:HG3	1:D:2059:ARG:NH2	2.28	0.48
1:D:2518:THR:HB	1:D:2519:ASP:OD2	2.14	0.48
1:A:1526:LYS:HG3	1:A:1560:SER:HB2	1.96	0.48
1:B:842:ALA:HB2	1:B:852:VAL:HG21	1.96	0.48
1:C:726:TRP:NE1	1:C:785:VAL:HG22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:TRP:NE1	1:D:785:VAL:HG22	2.29	0.48
1:D:2456:ILE:HG23	1:D:2524:LEU:HD21	1.96	0.48
1:E:267:PHE:HB3	1:E:271:ILE:HB	1.96	0.48
1:E:2056:MET:HG3	1:E:2059:ARG:NH2	2.28	0.48
1:A:206:ILE:HG23	1:A:922:MET:HE3	1.96	0.47
1:A:1577:LYS:NZ	1:A:1581:GLY:HA2	2.29	0.47
1:B:2367:ARG:HH12	1:B:2423:LEU:HD22	1.79	0.47
1:B:2426:PHE:HD2	1:B:2505:ASN:HD22	1.62	0.47
1:B:2456:ILE:HG23	1:B:2524:LEU:HD21	1.96	0.47
1:C:267:PHE:HB3	1:C:271:ILE:HB	1.96	0.47
1:E:126:ALA:HB2	1:E:997:ILE:HD11	1.94	0.47
1:E:2270:ALA:O	1:E:2273:GLU:HG3	2.14	0.47
1:A:267:PHE:HB3	1:A:271:ILE:HB	1.96	0.47
1:A:842:ALA:HB2	1:A:852:VAL:HG21	1.96	0.47
1:A:1622:ARG:HD2	1:A:1715:PRO:HB3	1.95	0.47
1:B:1577:LYS:NZ	1:B:1581:GLY:HA2	2.29	0.47
1:B:2242:ALA:O	1:B:2245:GLU:HG3	2.14	0.47
1:D:337:THR:HB	1:D:430:GLY:HA2	1.95	0.47
1:D:2361:ARG:HD3	1:E:2498:PRO:HG3	1.95	0.47
1:A:26:GLN:HA	1:A:57:LYS:HZ1	1.79	0.47
1:A:1457:PHE:CZ	1:A:1471:VAL:HG22	2.50	0.47
1:A:2056:MET:HA	1:A:2059:ARG:HD3	1.97	0.47
1:B:1526:LYS:HG3	1:B:1560:SER:HB2	1.96	0.47
1:B:1622:ARG:HD2	1:B:1715:PRO:HB3	1.95	0.47
1:C:1167:HIS:ND1	1:C:1199:PHE:HB3	2.28	0.47
1:D:1167:HIS:ND1	1:D:1199:PHE:HB3	2.28	0.47
1:D:2235:GLY:O	1:D:2239:GLN:HG2	2.15	0.47
1:D:2426:PHE:HD2	1:D:2505:ASN:HD22	1.61	0.47
1:E:206:ILE:HG23	1:E:922:MET:HE3	1.96	0.47
1:E:2518:THR:HB	1:E:2519:ASP:OD2	2.13	0.47
1:A:409:TYR:CD2	1:A:410:LYS:HD2	2.49	0.47
1:A:2107:ARG:O	1:A:2111:GLU:HG2	2.14	0.47
1:B:267:PHE:HB3	1:B:271:ILE:HB	1.96	0.47
1:B:2525:LEU:HA	1:B:2528:LEU:HB3	1.95	0.47
1:C:409:TYR:CD2	1:C:410:LYS:HD2	2.49	0.47
1:D:1457:PHE:CZ	1:D:1471:VAL:HG22	2.50	0.47
1:E:53:THR:O	1:E:57:LYS:HG2	2.15	0.47
1:E:266:ASN:HD22	1:E:446:LEU:HD22	1.78	0.47
1:E:1249:TYR:HB3	1:E:1265:VAL:HG22	1.96	0.47
1:E:1757:LEU:HB2	1:E:1787:ILE:HD11	1.97	0.47
1:E:2456:ILE:HG23	1:E:2524:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:TYR:HB3	1:A:1265:VAL:HG22	1.96	0.47
1:A:2235:GLY:O	1:A:2239:GLN:HG2	2.15	0.47
1:C:1647:MET:HE1	1:C:1856:ARG:N	2.28	0.47
1:C:2235:GLY:O	1:C:2239:GLN:HG2	2.15	0.47
1:D:70:ARG:HH12	1:D:1883:MET:CE	2.28	0.47
1:D:2270:ALA:O	1:D:2273:GLU:HG3	2.14	0.47
1:E:1123:ARG:HD3	1:E:1140:TRP:HE3	1.80	0.47
1:E:1526:LYS:HG3	1:E:1560:SER:HB2	1.96	0.47
1:B:70:ARG:HH12	1:B:1883:MET:CE	2.28	0.47
1:B:337:THR:HB	1:B:430:GLY:HA2	1.95	0.47
1:C:1526:LYS:HG3	1:C:1560:SER:HB2	1.96	0.47
1:D:504:GLN:HA	1:D:507:ASN:ND2	2.30	0.47
1:E:504:GLN:HA	1:E:507:ASN:ND2	2.30	0.47
1:A:2074:LEU:HA	1:A:2077:MET:HG3	1.97	0.47
1:A:2270:ALA:O	1:A:2273:GLU:HG3	2.14	0.47
1:B:504:GLN:HA	1:B:507:ASN:ND2	2.29	0.47
1:B:1167:HIS:ND1	1:B:1199:PHE:HB3	2.28	0.47
1:B:1457:PHE:CZ	1:B:1471:VAL:HG22	2.50	0.47
1:B:2109:VAL:HA	1:B:2112:VAL:HG22	1.97	0.47
1:B:2195:SER:HA	1:B:2198:VAL:HG22	1.97	0.47
1:C:2195:SER:HA	1:C:2198:VAL:HG22	1.97	0.47
1:C:2367:ARG:HH12	1:C:2423:LEU:HD22	1.79	0.47
1:C:2525:LEU:HA	1:C:2528:LEU:HB3	1.95	0.47
1:E:2242:ALA:O	1:E:2245:GLU:HG3	2.14	0.47
1:A:504:GLN:HA	1:A:507:ASN:ND2	2.29	0.47
1:A:2456:ILE:HG23	1:A:2524:LEU:HD21	1.96	0.47
1:B:219:ALA:HA	1:B:222:ARG:HE	1.80	0.47
1:C:219:ALA:HA	1:C:222:ARG:HE	1.80	0.47
1:C:2103:ARG:HB3	1:D:2256:MET:HE3	1.96	0.47
1:C:2107:ARG:O	1:C:2111:GLU:HG2	2.14	0.47
1:C:2109:VAL:HA	1:C:2112:VAL:HG22	1.97	0.47
1:C:2242:ALA:O	1:C:2245:GLU:HG3	2.14	0.47
1:D:206:ILE:HG23	1:D:922:MET:HE3	1.96	0.47
1:D:267:PHE:HB3	1:D:271:ILE:HB	1.96	0.47
1:A:53:THR:O	1:A:57:LYS:HG2	2.15	0.47
1:B:1319:PRO:HG2	1:B:1591:LEU:HD11	1.97	0.47
1:B:1937:GLN:HG2	1:C:294:GLN:NE2	2.30	0.47
1:C:2426:PHE:HD2	1:C:2505:ASN:HD22	1.61	0.47
1:D:1060:LEU:HA	1:D:1063:ILE:HG22	1.97	0.47
1:D:1310:TYR:CE1	1:D:1603:ILE:HD12	2.50	0.47
1:D:1639:THR:HG22	1:D:1640:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2109:VAL:HA	1:D:2112:VAL:HG22	1.97	0.47
1:D:2525:LEU:HA	1:D:2528:LEU:HB3	1.95	0.47
1:E:2112:VAL:HG21	1:E:2251:ARG:HA	1.97	0.47
1:A:219:ALA:HA	1:A:222:ARG:HE	1.80	0.47
1:A:1310:TYR:CE1	1:A:1603:ILE:HD12	2.50	0.47
1:A:1639:THR:HG22	1:A:1640:GLY:N	2.30	0.47
1:A:2109:VAL:HA	1:A:2112:VAL:HG22	1.97	0.47
1:A:2404:GLY:HA3	1:A:2419:ARG:HE	1.80	0.47
1:B:1123:ARG:HD3	1:B:1140:TRP:HE3	1.80	0.47
1:B:2168:ALA:HA	1:E:1117:LEU:HD11	1.95	0.47
1:C:1622:ARG:HD2	1:C:1715:PRO:HB3	1.95	0.47
1:C:2112:VAL:HG21	1:C:2251:ARG:HA	1.97	0.47
1:D:53:THR:O	1:D:57:LYS:HG2	2.15	0.47
1:D:1123:ARG:HD3	1:D:1140:TRP:HE3	1.80	0.47
1:D:2100:GLN:HB2	1:E:2260:TYR:CD2	2.48	0.47
1:E:2107:ARG:O	1:E:2111:GLU:HG2	2.14	0.47
1:E:2109:VAL:HA	1:E:2112:VAL:HG22	1.97	0.47
1:A:1757:LEU:HB2	1:A:1787:ILE:HD11	1.96	0.46
1:A:2242:ALA:O	1:A:2245:GLU:HG3	2.14	0.46
1:A:2472:CYS:SG	1:A:2498:PRO:HA	2.55	0.46
1:C:25:LEU:HA	1:C:27:TYR:HB2	1.97	0.46
1:C:504:GLN:HA	1:C:507:ASN:ND2	2.29	0.46
1:D:1249:TYR:HB3	1:D:1265:VAL:HG22	1.97	0.46
1:E:70:ARG:HH12	1:E:1883:MET:CE	2.28	0.46
1:E:2235:GLY:O	1:E:2239:GLN:HG2	2.15	0.46
1:E:2404:GLY:HA3	1:E:2419:ARG:HE	1.80	0.46
1:B:813:PHE:O	1:B:817:ILE:HG12	2.15	0.46
1:C:206:ILE:HG23	1:C:922:MET:HE3	1.96	0.46
1:C:1123:ARG:HD3	1:C:1140:TRP:HE3	1.80	0.46
1:C:2066:GLN:HA	1:C:2069:GLN:CD	2.41	0.46
1:D:1526:LYS:HG3	1:D:1560:SER:HB2	1.96	0.46
1:D:2112:VAL:HG21	1:D:2251:ARG:HA	1.97	0.46
1:D:2195:SER:HA	1:D:2198:VAL:HG22	1.97	0.46
1:E:219:ALA:HA	1:E:222:ARG:HE	1.80	0.46
1:E:489:THR:HG23	1:E:503:ALA:HB3	1.97	0.46
1:E:1639:THR:HG22	1:E:1640:GLY:N	2.30	0.46
1:A:2458:ALA:HB1	1:A:2512:LEU:HD11	1.97	0.46
1:B:2066:GLN:HA	1:B:2069:GLN:CD	2.41	0.46
1:B:2074:LEU:HA	1:B:2077:MET:HG3	1.97	0.46
1:B:2235:GLY:O	1:B:2239:GLN:HG2	2.15	0.46
1:C:1115:GLU:OE2	1:C:1117:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1757:LEU:HB2	1:C:1787:ILE:HD11	1.97	0.46
1:C:1937:GLN:HE21	1:D:290:LEU:HD11	1.80	0.46
1:C:2270:ALA:O	1:C:2273:GLU:HG3	2.14	0.46
1:D:25:LEU:HA	1:D:27:TYR:HB2	1.98	0.46
1:E:1319:PRO:HG2	1:E:1591:LEU:HD11	1.97	0.46
1:A:2066:GLN:HA	1:A:2069:GLN:CD	2.41	0.46
1:A:2195:SER:HA	1:A:2198:VAL:HG22	1.97	0.46
1:B:1060:LEU:HA	1:B:1063:ILE:HG22	1.97	0.46
1:B:1249:TYR:HB3	1:B:1265:VAL:HG22	1.97	0.46
1:B:1341:ILE:HG21	1:B:1357:LEU:HB3	1.98	0.46
1:B:2056:MET:HA	1:B:2059:ARG:HD3	1.97	0.46
1:C:1187:VAL:CG1	1:D:1179:ASN:HD21	2.27	0.46
1:C:2093:GLN:HG2	1:D:2267:HIS:HB2	1.97	0.46
1:D:1757:LEU:HB2	1:D:1787:ILE:HD11	1.97	0.46
1:D:2367:ARG:HH12	1:D:2423:LEU:HD22	1.79	0.46
1:E:1310:TYR:CE1	1:E:1603:ILE:HD12	2.50	0.46
1:E:2367:ARG:HH12	1:E:2423:LEU:HD22	1.80	0.46
1:A:70:ARG:HH12	1:A:1883:MET:CE	2.28	0.46
1:A:813:PHE:O	1:A:817:ILE:HG12	2.16	0.46
1:A:2100:GLN:HB2	1:B:2260:TYR:HD2	1.81	0.46
1:A:2191:ALA:HB3	1:D:1151:ASN:HD21	1.80	0.46
1:B:53:THR:O	1:B:57:LYS:HG2	2.15	0.46
1:B:1639:THR:HG22	1:B:1640:GLY:N	2.30	0.46
1:C:489:THR:HG23	1:C:503:ALA:HB3	1.98	0.46
1:C:1457:PHE:CZ	1:C:1471:VAL:HG22	2.50	0.46
1:D:14:THR:C	1:D:15:ARG:HD3	2.41	0.46
1:D:813:PHE:O	1:D:817:ILE:HG12	2.15	0.46
1:D:2158:GLN:NE2	1:E:2199:MET:HE2	2.20	0.46
1:D:2458:ALA:HB1	1:D:2512:LEU:HD11	1.97	0.46
1:E:25:LEU:HA	1:E:27:TYR:HB2	1.98	0.46
1:E:547:ASP:HB3	1:E:550:GLU:HB2	1.98	0.46
1:A:25:LEU:HA	1:A:27:TYR:HB2	1.97	0.46
1:A:2054:PRO:O	1:A:2058:GLU:OE1	2.34	0.46
1:B:2054:PRO:O	1:B:2058:GLU:OE1	2.34	0.46
1:B:2438:GLN:O	1:B:2537:TYR:HB2	2.16	0.46
1:C:14:THR:C	1:C:15:ARG:HD3	2.41	0.46
1:C:53:THR:O	1:C:57:LYS:HG2	2.15	0.46
1:C:547:ASP:HB3	1:C:550:GLU:HB2	1.98	0.46
1:C:1341:ILE:HG21	1:C:1357:LEU:HB3	1.98	0.46
1:C:1639:THR:HG22	1:C:1640:GLY:N	2.30	0.46
1:C:2056:MET:HA	1:C:2059:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2074:LEU:HA	1:C:2077:MET:HG3	1.97	0.46
1:D:489:THR:HG23	1:D:503:ALA:HB3	1.97	0.46
1:D:1115:GLU:OE2	1:D:1117:LEU:HD23	2.15	0.46
1:D:1937:GLN:NE2	1:E:290:LEU:HD11	2.29	0.46
1:E:1457:PHE:CZ	1:E:1471:VAL:HG22	2.50	0.46
1:A:2457:ARG:HD2	1:E:2428:ASP:O	2.16	0.46
1:B:414:LYS:HD2	1:B:414:LYS:HA	1.79	0.46
1:B:489:THR:HG23	1:B:503:ALA:HB3	1.98	0.46
1:B:855:ALA:HB1	1:B:873:VAL:HG13	1.98	0.46
1:B:2240:MET:HA	1:B:2243:GLN:HB2	1.98	0.46
1:C:855:ALA:HB1	1:C:873:VAL:HG13	1.98	0.46
1:C:2240:MET:HA	1:C:2243:GLN:HB2	1.98	0.46
1:D:547:ASP:HB3	1:D:550:GLU:HB2	1.98	0.46
1:D:1324:MET:HE3	1:D:1574:PHE:CZ	2.51	0.46
1:D:2240:MET:HA	1:D:2243:GLN:HB2	1.98	0.46
1:A:547:ASP:HB3	1:A:550:GLU:HB2	1.98	0.46
1:A:844:VAL:HG12	1:A:845:MET:HE2	1.98	0.46
1:A:2112:VAL:HG21	1:A:2251:ARG:HA	1.97	0.46
1:A:2367:ARG:HH12	1:A:2423:LEU:HD22	1.79	0.46
1:B:14:THR:C	1:B:15:ARG:HD3	2.41	0.46
1:B:25:LEU:HA	1:B:27:TYR:HB2	1.98	0.46
1:B:844:VAL:HG12	1:B:845:MET:HE2	1.98	0.46
1:B:1310:TYR:CE1	1:B:1603:ILE:HD12	2.50	0.46
1:C:217:LEU:HD21	1:C:238:ILE:HD11	1.98	0.46
1:C:1214:ILE:HG22	1:C:1217:GLN:HB2	1.98	0.46
1:D:2056:MET:HA	1:D:2059:ARG:HD3	1.97	0.46
1:D:2066:GLN:HA	1:D:2069:GLN:CD	2.41	0.46
1:D:2472:CYS:SG	1:D:2498:PRO:HA	2.55	0.46
1:E:14:THR:C	1:E:15:ARG:HD3	2.41	0.46
1:E:2074:LEU:HA	1:E:2077:MET:HG3	1.97	0.46
1:A:351:TYR:HB2	1:A:409:TYR:CE1	2.51	0.46
1:A:855:ALA:HB1	1:A:873:VAL:HG13	1.98	0.46
1:A:2302:LEU:HD22	1:E:2353:LYS:HD2	1.98	0.46
1:B:1115:GLU:OE2	1:B:1117:LEU:HD23	2.15	0.46
1:B:1324:MET:HE3	1:B:1574:PHE:CZ	2.51	0.46
1:C:70:ARG:HH12	1:C:1883:MET:CE	2.28	0.46
1:C:813:PHE:O	1:C:817:ILE:HG12	2.16	0.46
1:C:1892:ARG:HD3	1:C:1892:ARG:HA	1.69	0.46
1:C:1921:VAL:HG11	1:D:995:LEU:HD13	1.96	0.46
1:C:2472:CYS:SG	1:C:2498:PRO:HA	2.55	0.46
1:D:2205:ALA:HA	1:D:2208:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLN:HA	1:E:57:LYS:HZ1	1.81	0.46
1:E:2056:MET:HA	1:E:2059:ARG:HD3	1.97	0.46
1:E:2195:SER:HA	1:E:2198:VAL:HG22	1.97	0.46
1:E:2472:CYS:SG	1:E:2498:PRO:HA	2.55	0.46
1:B:217:LEU:HD21	1:B:238:ILE:HD11	1.98	0.46
1:B:2112:VAL:HG21	1:B:2251:ARG:HA	1.97	0.46
1:B:2404:GLY:HA3	1:B:2419:ARG:HE	1.80	0.46
1:C:854:GLN:HE21	1:D:549:ASP:HA	1.81	0.46
1:C:1060:LEU:HA	1:C:1063:ILE:HG22	1.97	0.46
1:C:2166:SER:HB2	1:C:2198:VAL:CG1	2.46	0.46
1:C:2438:GLN:O	1:C:2537:TYR:HB2	2.16	0.46
1:D:855:ALA:HB1	1:D:873:VAL:HG13	1.98	0.46
1:D:1341:ILE:HG21	1:D:1357:LEU:HB3	1.98	0.46
1:D:1968:VAL:HG12	1:D:1970:LYS:H	1.81	0.46
1:D:2074:LEU:HA	1:D:2077:MET:HG3	1.97	0.46
1:D:2166:SER:HB2	1:D:2198:VAL:CG1	2.46	0.46
1:E:351:TYR:HB2	1:E:409:TYR:CE1	2.51	0.46
1:E:1115:GLU:OE2	1:E:1117:LEU:HD23	2.15	0.46
1:E:1214:ILE:HG22	1:E:1217:GLN:HB2	1.98	0.46
1:E:1324:MET:HE3	1:E:1574:PHE:CZ	2.51	0.46
1:E:1681:PHE:CD1	1:E:1702:LEU:HG	2.51	0.46
1:E:2458:ALA:HB1	1:E:2512:LEU:HD11	1.97	0.46
1:A:489:THR:HG23	1:A:503:ALA:HB3	1.98	0.45
1:A:1055:MET:O	1:A:1058:GLU:HG3	2.17	0.45
1:A:1519:ILE:HG12	1:A:1574:PHE:HD1	1.81	0.45
1:A:1634:VAL:HG22	1:B:1202:HIS:CE1	2.51	0.45
1:A:2071:GLY:O	1:A:2074:LEU:HG	2.16	0.45
1:B:351:TYR:HB2	1:B:409:TYR:CE1	2.51	0.45
1:B:1968:VAL:HG12	1:B:1970:LYS:H	1.81	0.45
1:B:2205:ALA:HA	1:B:2208:TYR:CD2	2.51	0.45
1:C:1310:TYR:CE1	1:C:1603:ILE:HD12	2.50	0.45
1:C:1670:TYR:CD1	1:C:1679:ARG:HG2	2.51	0.45
1:D:351:TYR:HB2	1:D:409:TYR:CE1	2.51	0.45
1:E:1670:TYR:CD1	1:E:1679:ARG:HG2	2.51	0.45
1:A:1123:ARG:HD3	1:A:1140:TRP:HE3	1.80	0.45
1:A:1163:ARG:O	1:A:1164:GLU:HG3	2.17	0.45
1:A:1341:ILE:HG21	1:A:1357:LEU:HB3	1.98	0.45
1:A:1968:VAL:HG12	1:A:1970:LYS:H	1.81	0.45
1:A:2236:GLU:O	1:A:2239:GLN:HB2	2.17	0.45
1:A:2438:GLN:O	1:A:2537:TYR:HB2	2.16	0.45
1:B:1055:MET:O	1:B:1058:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1163:ARG:O	1:B:1164:GLU:HG3	2.17	0.45
1:B:1671:ASP:HB3	1:B:1674:GLU:HB3	1.99	0.45
1:B:1757:LEU:HB2	1:B:1787:ILE:HD11	1.97	0.45
1:B:2236:GLU:O	1:B:2239:GLN:HB2	2.17	0.45
1:B:2364:GLU:HB3	1:C:2487:PHE:CZ	2.51	0.45
1:B:2458:ALA:HB1	1:B:2512:LEU:HD11	1.97	0.45
1:C:1163:ARG:O	1:C:1164:GLU:HG3	2.17	0.45
1:C:1249:TYR:HB3	1:C:1265:VAL:HG22	1.97	0.45
1:C:1671:ASP:HB3	1:C:1674:GLU:HB3	1.99	0.45
1:D:219:ALA:HA	1:D:222:ARG:HE	1.80	0.45
1:D:1319:PRO:HG2	1:D:1591:LEU:HD11	1.97	0.45
1:D:2054:PRO:O	1:D:2058:GLU:OE1	2.34	0.45
1:D:2404:GLY:HA3	1:D:2419:ARG:HE	1.81	0.45
1:E:1519:ILE:HG12	1:E:1574:PHE:HD1	1.81	0.45
1:E:2071:GLY:O	1:E:2074:LEU:HG	2.16	0.45
1:E:2205:ALA:HA	1:E:2208:TYR:CD2	2.51	0.45
1:A:1681:PHE:CD1	1:A:1702:LEU:HG	2.51	0.45
1:A:2205:ALA:HA	1:A:2208:TYR:CD2	2.51	0.45
1:C:1319:PRO:HG2	1:C:1591:LEU:HD11	1.97	0.45
1:C:1324:MET:HE3	1:C:1574:PHE:CZ	2.51	0.45
1:C:1968:VAL:HG12	1:C:1970:LYS:H	1.81	0.45
1:C:2205:ALA:HA	1:C:2208:TYR:CD2	2.51	0.45
1:D:217:LEU:HD21	1:D:238:ILE:HD11	1.98	0.45
1:D:1670:TYR:CD1	1:D:1679:ARG:HG2	2.51	0.45
1:E:217:LEU:HD21	1:E:238:ILE:HD11	1.98	0.45
1:A:14:THR:C	1:A:15:ARG:HD3	2.41	0.45
1:A:1060:LEU:HA	1:A:1063:ILE:HG22	1.97	0.45
1:A:1177:ALA:HB2	1:A:1188:GLU:O	2.17	0.45
1:A:1324:MET:HE3	1:A:1574:PHE:CZ	2.51	0.45
1:A:2287:TRP:HH2	1:B:682:ASN:HD21	1.64	0.45
1:B:504:GLN:HA	1:B:507:ASN:HD21	1.82	0.45
1:C:1519:ILE:HG12	1:C:1574:PHE:HD1	1.81	0.45
1:C:2236:GLU:O	1:C:2239:GLN:HB2	2.17	0.45
1:D:1519:ILE:HG12	1:D:1574:PHE:HD1	1.81	0.45
1:D:2236:GLU:O	1:D:2239:GLN:HB2	2.17	0.45
1:E:899:VAL:HG13	1:E:904:LYS:HB2	1.98	0.45
1:E:2066:GLN:HA	1:E:2069:GLN:CD	2.41	0.45
1:E:2240:MET:HA	1:E:2243:GLN:HB2	1.98	0.45
1:A:504:GLN:HA	1:A:507:ASN:HD21	1.82	0.45
1:A:1319:PRO:HG2	1:A:1591:LEU:HD11	1.97	0.45
1:B:1214:ILE:HG22	1:B:1217:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:TRP:HZ2	1:B:1773:VAL:HG11	1.82	0.45
1:B:2270:ALA:O	1:B:2273:GLU:HG3	2.14	0.45
1:B:2472:CYS:SG	1:B:2498:PRO:HA	2.55	0.45
1:D:1681:PHE:CD1	1:D:1702:LEU:HG	2.51	0.45
1:E:1163:ARG:O	1:E:1164:GLU:HG3	2.17	0.45
1:E:2236:GLU:O	1:E:2239:GLN:HB2	2.17	0.45
1:A:1115:GLU:OE2	1:A:1117:LEU:HD23	2.15	0.45
1:A:1741:TRP:HZ2	1:A:1773:VAL:HG11	1.82	0.45
1:A:2240:MET:HA	1:A:2243:GLN:HB2	1.98	0.45
1:B:547:ASP:HB3	1:B:550:GLU:HB2	1.98	0.45
1:C:828:LEU:HD12	1:C:831:LEU:HD23	1.99	0.45
1:C:844:VAL:HG12	1:C:845:MET:HE2	1.98	0.45
1:D:899:VAL:HG13	1:D:904:LYS:HB2	1.98	0.45
1:D:1925:GLU:HG2	1:E:1004:ILE:HD13	1.97	0.45
1:E:813:PHE:O	1:E:817:ILE:HG12	2.16	0.45
1:E:855:ALA:HB1	1:E:873:VAL:HG13	1.98	0.45
1:E:2054:PRO:O	1:E:2058:GLU:OE1	2.34	0.45
1:A:217:LEU:HD21	1:A:238:ILE:HD11	1.98	0.45
1:A:1670:TYR:CD1	1:A:1679:ARG:HG2	2.51	0.45
1:A:2146:GLN:HE21	1:D:1067:LYS:HD2	1.82	0.45
1:A:2204:THR:HA	1:A:2207:GLN:OE1	2.17	0.45
1:C:218:SER:O	1:C:222:ARG:HG3	2.17	0.45
1:C:504:GLN:HA	1:C:507:ASN:HD21	1.82	0.45
1:D:1163:ARG:O	1:D:1164:GLU:HG3	2.17	0.45
1:D:1881:ASP:HB3	1:D:1884:HIS:ND1	2.32	0.45
1:E:1968:VAL:HG12	1:E:1970:LYS:H	1.81	0.45
1:A:351:TYR:HB2	1:A:409:TYR:HE1	1.82	0.45
1:B:311:TYR:HB3	1:B:312:VAL:H	1.59	0.45
1:B:1060:LEU:HG	1:C:2147:ARG:NH1	2.32	0.45
1:B:1670:TYR:CD1	1:B:1679:ARG:HG2	2.51	0.45
1:B:1681:PHE:CD1	1:B:1702:LEU:HG	2.51	0.45
1:C:1055:MET:O	1:C:1058:GLU:HG3	2.17	0.45
1:C:1681:PHE:CD1	1:C:1702:LEU:HG	2.51	0.45
1:C:2111:GLU:CD	1:D:2250:ARG:HG3	2.42	0.45
1:D:1214:ILE:HG22	1:D:1214:ILE:O	2.17	0.45
1:D:1214:ILE:HG22	1:D:1217:GLN:HB2	1.98	0.45
1:D:1741:TRP:HZ2	1:D:1773:VAL:HG11	1.82	0.45
1:D:1745:PHE:HB2	1:D:1758:ILE:HB	1.99	0.45
1:D:2438:GLN:O	1:D:2537:TYR:HB2	2.16	0.45
1:E:1060:LEU:HA	1:E:1063:ILE:HG22	1.97	0.45
1:E:1881:ASP:HB3	1:E:1884:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:ALA:HB2	1:B:1188:GLU:O	2.17	0.45
1:B:1519:ILE:HG12	1:B:1574:PHE:HD1	1.81	0.45
1:B:1881:ASP:HB3	1:B:1884:HIS:ND1	2.32	0.45
1:C:1745:PHE:HB2	1:C:1758:ILE:HB	1.99	0.45
1:C:2054:PRO:O	1:C:2058:GLU:OE1	2.34	0.45
1:C:2204:THR:HA	1:C:2207:GLN:OE1	2.17	0.45
1:C:2458:ALA:HB1	1:C:2512:LEU:HD11	1.97	0.45
1:E:2438:GLN:O	1:E:2537:TYR:HB2	2.16	0.45
1:A:2166:SER:HB2	1:A:2198:VAL:CG1	2.46	0.45
1:B:899:VAL:HG13	1:B:904:LYS:HB2	1.98	0.45
1:B:2071:GLY:O	1:B:2074:LEU:HG	2.16	0.45
1:B:2140:ASP:CG	1:B:2141:ILE:HG13	2.42	0.45
1:C:2404:GLY:HA3	1:C:2419:ARG:HE	1.80	0.45
1:D:844:VAL:HG12	1:D:845:MET:HE2	1.98	0.45
1:E:844:VAL:HG12	1:E:845:MET:HE2	1.98	0.45
1:E:1214:ILE:HG22	1:E:1214:ILE:O	2.17	0.45
1:E:1341:ILE:HG21	1:E:1357:LEU:HB3	1.98	0.45
1:B:828:LEU:HD12	1:B:831:LEU:HD23	1.99	0.44
1:B:1511:GLY:HA3	1:B:1579:LYS:HE2	1.99	0.44
1:B:2166:SER:HB2	1:B:2198:VAL:CG1	2.46	0.44
1:C:351:TYR:HB2	1:C:409:TYR:CE1	2.51	0.44
1:C:1511:GLY:HA3	1:C:1579:LYS:HE2	1.99	0.44
1:C:2071:GLY:O	1:C:2074:LEU:HG	2.16	0.44
1:C:2140:ASP:CG	1:C:2141:ILE:HG13	2.42	0.44
1:D:504:GLN:HA	1:D:507:ASN:HD21	1.82	0.44
1:D:828:LEU:HD12	1:D:831:LEU:HD23	1.99	0.44
1:D:1055:MET:O	1:D:1058:GLU:HG3	2.17	0.44
1:D:2204:THR:HA	1:D:2207:GLN:OE1	2.17	0.44
1:E:504:GLN:HA	1:E:507:ASN:HD21	1.82	0.44
1:A:218:SER:O	1:A:222:ARG:HG3	2.17	0.44
1:B:218:SER:O	1:B:222:ARG:HG3	2.17	0.44
1:B:2158:GLN:O	1:C:2199:MET:HE1	2.17	0.44
1:B:2204:THR:HA	1:B:2207:GLN:OE1	2.17	0.44
1:D:2083:ALA:O	1:D:2086:LEU:HG	2.17	0.44
1:E:192:ARG:HD2	1:E:265:GLN:HG2	2.00	0.44
1:E:1671:ASP:HB3	1:E:1674:GLU:HB3	1.99	0.44
1:E:1882:PRO:O	1:E:1885:TYR:HB2	2.17	0.44
1:E:2166:SER:HB2	1:E:2198:VAL:CG1	2.46	0.44
1:A:1100:VAL:HB	1:A:1596:VAL:HG22	1.99	0.44
1:A:1214:ILE:O	1:A:1214:ILE:HG22	2.17	0.44
1:B:351:TYR:HB2	1:B:409:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.85	0.44
1:C:1577:LYS:HZ3	1:C:1581:GLY:HA2	1.82	0.44
1:C:2112:VAL:O	1:C:2116:ILE:HG23	2.17	0.44
1:D:7:LEU:O	1:D:11:ILE:HG12	2.18	0.44
1:D:827:THR:HA	1:D:830:MET:SD	2.58	0.44
1:D:1671:ASP:HB3	1:D:1674:GLU:HB3	1.99	0.44
1:D:2368:THR:HB	1:E:2455:ASP:OD1	2.17	0.44
1:E:351:TYR:HB2	1:E:409:TYR:HE1	1.82	0.44
1:E:2083:ALA:O	1:E:2086:LEU:HG	2.17	0.44
1:A:192:ARG:HD2	1:A:265:GLN:HG2	2.00	0.44
1:A:827:THR:HA	1:A:830:MET:SD	2.58	0.44
1:B:119:LEU:HB2	1:B:990:ILE:HD11	1.99	0.44
1:B:708:ILE:HA	1:B:711:THR:HG22	2.00	0.44
1:C:783:VAL:HG22	1:C:832:ARG:NE	2.33	0.44
1:C:1078:LYS:HE2	1:D:1202:HIS:HB3	1.99	0.44
1:D:1455:PHE:CE1	1:D:1478:ASP:HB3	2.52	0.44
1:D:1651:ARG:HA	1:D:1856:ARG:NH1	2.33	0.44
1:D:1680:TRP:HZ3	1:D:1682:LYS:HG3	1.83	0.44
1:E:218:SER:O	1:E:222:ARG:HG3	2.17	0.44
1:E:1892:ARG:HD3	1:E:1892:ARG:HA	1.69	0.44
1:E:2140:ASP:CG	1:E:2141:ILE:HG13	2.42	0.44
1:A:1214:ILE:HG22	1:A:1217:GLN:HB2	1.98	0.44
1:A:1511:GLY:HA3	1:A:1579:LYS:HE2	1.99	0.44
1:A:1882:PRO:O	1:A:1885:TYR:HB2	2.18	0.44
1:A:2140:ASP:CG	1:A:2141:ILE:HG13	2.42	0.44
1:B:655:ILE:HG21	1:B:660:ILE:HD13	2.00	0.44
1:B:1651:ARG:HA	1:B:1856:ARG:NH1	2.33	0.44
1:B:2191:ALA:HB3	1:E:1151:ASN:HD21	1.82	0.44
1:C:119:LEU:HB2	1:C:990:ILE:HD11	2.00	0.44
1:C:1214:ILE:HG22	1:C:1214:ILE:O	2.17	0.44
1:C:1881:ASP:HB3	1:C:1884:HIS:ND1	2.32	0.44
1:D:655:ILE:HG21	1:D:660:ILE:HD13	2.00	0.44
1:E:827:THR:HA	1:E:830:MET:SD	2.58	0.44
1:E:1177:ALA:HB2	1:E:1188:GLU:O	2.17	0.44
1:A:1630:ALA:O	1:A:1634:VAL:HG23	2.18	0.44
1:A:1671:ASP:HB3	1:A:1674:GLU:HB3	1.99	0.44
1:A:1881:ASP:HB3	1:A:1884:HIS:ND1	2.32	0.44
1:A:2112:VAL:O	1:A:2116:ILE:HG23	2.17	0.44
1:B:783:VAL:HG22	1:B:832:ARG:NE	2.33	0.44
1:C:7:LEU:O	1:C:11:ILE:HG12	2.18	0.44
1:C:708:ILE:HA	1:C:711:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:LEU:O	1:C:864:LEU:HD12	2.18	0.44
1:C:899:VAL:HG13	1:C:904:LYS:HB2	1.98	0.44
1:C:1100:VAL:HB	1:C:1596:VAL:HG22	1.99	0.44
1:C:2083:ALA:O	1:C:2086:LEU:HG	2.17	0.44
1:C:2100:GLN:HB2	1:D:2260:TYR:HD2	1.83	0.44
1:C:2169:GLU:OE2	1:D:2193:ARG:HD3	2.17	0.44
1:D:256:GLU:HG3	1:D:439:TYR:CE1	2.53	0.44
1:D:1882:PRO:O	1:D:1885:TYR:HB2	2.18	0.44
1:D:2071:GLY:O	1:D:2074:LEU:HG	2.16	0.44
1:D:2112:VAL:O	1:D:2116:ILE:HG23	2.17	0.44
1:E:256:GLU:HG3	1:E:439:TYR:CE1	2.53	0.44
1:E:1455:PHE:CE1	1:E:1478:ASP:HB3	2.52	0.44
1:E:1511:GLY:HA3	1:E:1579:LYS:HE2	1.99	0.44
1:A:414:LYS:HD2	1:A:414:LYS:HA	1.80	0.44
1:A:899:VAL:HG13	1:A:904:LYS:HB2	1.98	0.44
1:A:2140:ASP:HB3	1:D:1067:LYS:HZ1	1.83	0.44
1:A:2181:LEU:HD21	1:B:2181:LEU:HD13	1.98	0.44
1:B:7:LEU:O	1:B:11:ILE:HG12	2.18	0.44
1:B:1680:TRP:HZ3	1:B:1682:LYS:HG3	1.83	0.44
1:B:2112:VAL:O	1:B:2116:ILE:HG23	2.17	0.44
1:C:1187:VAL:HG12	1:D:1179:ASN:ND2	2.30	0.44
1:C:1741:TRP:HZ2	1:C:1773:VAL:HG11	1.82	0.44
1:C:2034:VAL:HA	1:D:825:SER:OG	2.17	0.44
1:C:2145:GLU:CD	1:D:2217:GLU:HG2	2.42	0.44
1:D:1895:ASP:O	1:D:1899:LEU:HD23	2.18	0.44
1:D:2056:MET:HA	1:D:2059:ARG:CD	2.48	0.44
1:E:414:LYS:HA	1:E:414:LYS:HD2	1.79	0.44
1:E:1100:VAL:HB	1:E:1596:VAL:HG22	1.99	0.44
1:E:1630:ALA:O	1:E:1634:VAL:HG23	2.18	0.44
1:E:1651:ARG:HA	1:E:1856:ARG:NH1	2.33	0.44
1:E:1680:TRP:HZ3	1:E:1682:LYS:HG3	1.83	0.44
1:E:2112:VAL:O	1:E:2116:ILE:HG23	2.17	0.44
1:A:1181:THR:OG1	1:A:1184:LYS:HB2	2.18	0.44
1:A:2227:GLU:HG2	1:A:2230:ARG:NH2	2.33	0.44
1:B:827:THR:HA	1:B:830:MET:SD	2.58	0.44
1:B:1745:PHE:HB2	1:B:1758:ILE:HB	1.99	0.44
1:B:2227:GLU:HG2	1:B:2230:ARG:NH2	2.33	0.44
1:C:687:ILE:HG13	1:C:691:MET:SD	2.58	0.44
1:C:2227:GLU:HG2	1:C:2230:ARG:NH2	2.33	0.44
1:D:218:SER:O	1:D:222:ARG:HG3	2.17	0.44
1:D:864:LEU:HD12	1:D:864:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1177:ALA:HB2	1:D:1188:GLU:O	2.17	0.44
1:E:864:LEU:HD12	1:E:864:LEU:O	2.18	0.44
1:E:1745:PHE:HB2	1:E:1758:ILE:HB	1.99	0.44
1:E:2227:GLU:HG2	1:E:2230:ARG:NH2	2.33	0.44
1:A:119:LEU:HB2	1:A:990:ILE:HD11	1.99	0.44
1:A:1455:PHE:CE1	1:A:1478:ASP:HB3	2.52	0.44
1:A:1651:ARG:HA	1:A:1856:ARG:NH1	2.33	0.44
1:A:1680:TRP:HZ3	1:A:1682:LYS:HG3	1.83	0.44
1:C:351:TYR:HB2	1:C:409:TYR:HE1	1.82	0.44
1:C:655:ILE:HG21	1:C:660:ILE:HD13	2.00	0.44
1:C:1455:PHE:CE1	1:C:1478:ASP:HB3	2.52	0.44
1:C:1680:TRP:HZ3	1:C:1682:LYS:HG3	1.83	0.44
1:D:26:GLN:HA	1:D:57:LYS:HZ1	1.83	0.44
1:D:351:TYR:HB2	1:D:409:TYR:HE1	1.82	0.44
1:D:2227:GLU:HG2	1:D:2230:ARG:NH2	2.33	0.44
1:E:1255:TYR:CE2	1:E:1296:ILE:HG22	2.52	0.44
1:A:655:ILE:HG21	1:A:660:ILE:HD13	2.00	0.43
1:A:1417:VAL:HG12	1:A:1426:ALA:HB3	2.00	0.43
1:B:864:LEU:HD12	1:B:864:LEU:O	2.18	0.43
1:B:1453:ARG:NE	1:B:1456:GLU:HB2	2.33	0.43
1:C:1177:ALA:HB2	1:C:1188:GLU:O	2.17	0.43
1:C:1651:ARG:HA	1:C:1856:ARG:NH1	2.33	0.43
1:D:2032:SER:C	1:D:2033:MET:HE2	2.43	0.43
1:D:2140:ASP:CG	1:D:2141:ILE:HG13	2.42	0.43
1:E:655:ILE:HG21	1:E:660:ILE:HD13	2.00	0.43
1:E:1895:ASP:O	1:E:1899:LEU:HD23	2.18	0.43
1:A:334:ARG:CZ	1:A:342:LYS:HA	2.48	0.43
1:A:828:LEU:HD12	1:A:831:LEU:HD23	1.99	0.43
1:A:1184:LYS:HD2	1:A:1184:LYS:O	2.19	0.43
1:A:1973:ARG:HH22	1:A:1976:ASN:CG	2.26	0.43
1:A:2083:ALA:O	1:A:2086:LEU:HG	2.17	0.43
1:B:256:GLU:HG3	1:B:439:TYR:CE1	2.53	0.43
1:B:1214:ILE:HG22	1:B:1214:ILE:O	2.17	0.43
1:B:1455:PHE:CE1	1:B:1478:ASP:HB3	2.52	0.43
1:B:2119:LEU:HD12	1:B:2119:LEU:HA	1.79	0.43
1:C:930:GLN:O	1:C:934:LEU:HD23	2.18	0.43
1:D:1973:ARG:HH22	1:D:1976:ASN:CG	2.26	0.43
1:E:7:LEU:O	1:E:11:ILE:HG12	2.18	0.43
1:E:828:LEU:HD12	1:E:831:LEU:HD23	1.99	0.43
1:E:1184:LYS:HD2	1:E:1184:LYS:O	2.18	0.43
1:E:2392:PHE:CD1	1:E:2398:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:HA	1:A:711:THR:HG22	2.00	0.43
1:A:1040:PRO:O	1:A:1044:ILE:HG12	2.18	0.43
1:B:1100:VAL:HB	1:B:1596:VAL:HG22	1.99	0.43
1:B:2083:ALA:O	1:B:2086:LEU:HG	2.17	0.43
1:C:732:PRO:HB3	1:C:763:VAL:HG21	2.00	0.43
1:C:1181:THR:OG1	1:C:1184:LYS:HB2	2.18	0.43
1:C:1184:LYS:O	1:C:1184:LYS:HD2	2.18	0.43
1:D:1630:ALA:O	1:D:1634:VAL:HG23	2.18	0.43
1:E:311:TYR:HB3	1:E:312:VAL:H	1.59	0.43
1:E:334:ARG:CZ	1:E:342:LYS:HA	2.48	0.43
1:E:737:ILE:HG22	1:E:741:MET:HE1	2.00	0.43
1:E:783:VAL:HG22	1:E:832:ARG:NE	2.33	0.43
1:E:1055:MET:O	1:E:1058:GLU:HG3	2.17	0.43
1:E:2204:THR:HA	1:E:2207:GLN:OE1	2.17	0.43
1:E:2364:GLU:HG3	1:E:2538:THR:HG22	2.01	0.43
1:A:1733:GLN:C	1:A:1735:ILE:H	2.26	0.43
1:B:750:ASN:HB3	1:B:753:GLU:HB2	2.00	0.43
1:B:1417:VAL:HG12	1:B:1426:ALA:HB3	2.00	0.43
1:B:1745:PHE:HB3	1:B:1758:ILE:HD12	2.01	0.43
1:C:26:GLN:HA	1:C:57:LYS:HZ1	1.83	0.43
1:C:1040:PRO:O	1:C:1044:ILE:HG12	2.18	0.43
1:C:1973:ARG:HH22	1:C:1976:ASN:CG	2.26	0.43
1:C:2056:MET:HA	1:C:2059:ARG:CD	2.48	0.43
1:D:334:ARG:CZ	1:D:342:LYS:HA	2.48	0.43
1:D:1511:GLY:HA3	1:D:1579:LYS:HE2	1.99	0.43
1:E:1163:ARG:C	1:E:1164:GLU:HG3	2.44	0.43
1:E:1745:PHE:HB3	1:E:1758:ILE:HD12	2.01	0.43
1:E:2056:MET:HA	1:E:2059:ARG:CD	2.48	0.43
1:A:2198:VAL:HA	1:A:2201:LEU:HG	2.00	0.43
1:B:687:ILE:HG13	1:B:691:MET:SD	2.58	0.43
1:B:2056:MET:HA	1:B:2059:ARG:CD	2.48	0.43
1:C:827:THR:HA	1:C:830:MET:SD	2.58	0.43
1:C:1630:ALA:O	1:C:1634:VAL:HG23	2.18	0.43
1:C:2148:ALA:HB2	1:D:2213:ILE:CD1	2.47	0.43
1:D:192:ARG:HD2	1:D:265:GLN:HG2	2.00	0.43
1:D:783:VAL:HG22	1:D:832:ARG:NE	2.33	0.43
1:D:930:GLN:O	1:D:934:LEU:HD23	2.19	0.43
1:A:1163:ARG:C	1:A:1164:GLU:HG3	2.44	0.43
1:A:1745:PHE:HB3	1:A:1758:ILE:HD12	2.01	0.43
1:A:2056:MET:HA	1:A:2059:ARG:CD	2.48	0.43
1:B:192:ARG:HD2	1:B:265:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1630:ALA:O	1:B:1634:VAL:HG23	2.18	0.43
1:C:450:LYS:HD3	1:C:478:ILE:HD12	2.01	0.43
1:C:750:ASN:HB3	1:C:753:GLU:HB2	2.00	0.43
1:C:2032:SER:C	1:C:2033:MET:HE2	2.43	0.43
1:D:1100:VAL:HB	1:D:1596:VAL:HG22	1.99	0.43
1:D:1184:LYS:HD2	1:D:1184:LYS:O	2.18	0.43
1:E:1040:PRO:O	1:E:1044:ILE:HG12	2.19	0.43
1:E:1741:TRP:HZ2	1:E:1773:VAL:HG11	1.82	0.43
1:A:256:GLU:HG3	1:A:439:TYR:CE1	2.53	0.43
1:A:2104:ILE:HG12	1:B:2256:MET:SD	2.59	0.43
1:A:2392:PHE:CD1	1:A:2398:GLY:HA3	2.54	0.43
1:B:1040:PRO:O	1:B:1044:ILE:HG12	2.18	0.43
1:B:1184:LYS:HD2	1:B:1184:LYS:O	2.19	0.43
1:B:1733:GLN:C	1:B:1735:ILE:H	2.26	0.43
1:B:1895:ASP:O	1:B:1899:LEU:HD23	2.18	0.43
1:B:2300:PHE:CE2	1:B:2331:TRP:HB2	2.54	0.43
1:C:334:ARG:CZ	1:C:342:LYS:HA	2.48	0.43
1:C:850:SER:CB	1:D:548:PRO:HB2	2.49	0.43
1:C:1882:PRO:O	1:C:1885:TYR:HB2	2.18	0.43
1:C:2198:VAL:HA	1:C:2201:LEU:HG	2.00	0.43
1:D:708:ILE:HA	1:D:711:THR:HG22	2.00	0.43
1:D:1122:TRP:CE2	1:D:1144:THR:HB	2.54	0.43
1:D:1446:VAL:HG13	1:D:1448:ASN:H	1.84	0.43
1:D:2392:PHE:CD1	1:D:2398:GLY:HA3	2.53	0.43
1:E:750:ASN:HB3	1:E:753:GLU:HB2	2.00	0.43
1:A:7:LEU:O	1:A:11:ILE:HG12	2.18	0.43
1:A:687:ILE:HG13	1:A:691:MET:SD	2.58	0.43
1:A:1745:PHE:HB2	1:A:1758:ILE:HB	1.99	0.43
1:B:450:LYS:HD3	1:B:478:ILE:HD12	2.01	0.43
1:B:1882:PRO:O	1:B:1885:TYR:HB2	2.18	0.43
1:B:1960:LEU:HD23	1:B:1960:LEU:HA	1.88	0.43
1:C:1122:TRP:CE2	1:C:1144:THR:HB	2.54	0.43
1:D:1214:ILE:O	1:D:1218:VAL:HG23	2.19	0.43
1:D:1453:ARG:NE	1:D:1456:GLU:HB2	2.33	0.43
1:D:1733:GLN:C	1:D:1735:ILE:H	2.26	0.43
1:D:1745:PHE:HB3	1:D:1758:ILE:HD12	2.01	0.43
1:D:1757:LEU:HD22	1:D:1760:ASP:HB3	2.01	0.43
1:D:2198:VAL:HA	1:D:2201:LEU:HG	2.00	0.43
1:E:680:LEU:HD23	1:E:744:VAL:HG13	2.01	0.43
1:E:2300:PHE:CE2	1:E:2331:TRP:HB2	2.54	0.43
1:A:864:LEU:HD12	1:A:864:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:CZ	1:B:342:LYS:HA	2.48	0.43
1:B:489:THR:HA	1:B:503:ALA:HB1	2.01	0.43
1:B:1181:THR:OG1	1:B:1184:LYS:HB2	2.18	0.43
1:B:1476:THR:O	1:B:1480:LYS:HG2	2.19	0.43
1:B:2456:ILE:HG12	1:B:2524:LEU:HD21	2.01	0.43
1:C:1162:PHE:CD2	1:C:1163:ARG:HG2	2.54	0.43
1:C:1453:ARG:NE	1:C:1456:GLU:HB2	2.33	0.43
1:C:2364:GLU:HG3	1:C:2538:THR:HG22	2.01	0.43
1:D:450:LYS:HD3	1:D:478:ILE:HD12	2.01	0.43
1:D:1163:ARG:C	1:D:1164:GLU:HG3	2.44	0.43
1:E:1162:PHE:CD2	1:E:1163:ARG:HG2	2.54	0.43
1:E:1181:THR:OG1	1:E:1184:LYS:HB2	2.18	0.43
1:E:1214:ILE:O	1:E:1218:VAL:HG23	2.19	0.43
1:A:783:VAL:HG22	1:A:832:ARG:NE	2.33	0.43
1:A:1453:ARG:NE	1:A:1456:GLU:HB2	2.33	0.43
1:A:1937:GLN:NE2	1:B:290:LEU:HD11	2.34	0.43
1:A:2032:SER:C	1:A:2033:MET:HE2	2.43	0.43
1:A:2300:PHE:CE2	1:A:2331:TRP:HB2	2.54	0.43
1:B:930:GLN:O	1:B:934:LEU:HD23	2.19	0.43
1:B:1255:TYR:CE2	1:B:1296:ILE:HG22	2.52	0.43
1:B:1608:GLU:HB2	1:B:1614:GLN:HG2	2.01	0.43
1:B:1973:ARG:HH22	1:B:1976:ASN:CG	2.26	0.43
1:C:192:ARG:HD2	1:C:265:GLN:HG2	2.00	0.43
1:C:256:GLU:HG3	1:C:439:TYR:CE1	2.53	0.43
1:C:1930:GLU:HB3	1:C:1994:TRP:CE2	2.54	0.43
1:C:2456:ILE:HG12	1:C:2524:LEU:HD21	2.01	0.43
1:D:1040:PRO:O	1:D:1044:ILE:HG12	2.18	0.43
1:D:1162:PHE:CD2	1:D:1163:ARG:HG2	2.54	0.43
1:D:2119:LEU:HD12	1:D:2119:LEU:HA	1.79	0.43
1:E:119:LEU:HB2	1:E:990:ILE:HD11	1.99	0.43
1:E:1973:ARG:HH22	1:E:1976:ASN:CG	2.26	0.43
1:A:1162:PHE:HE2	1:A:1272:GLY:HA2	1.84	0.42
1:A:2064:VAL:O	1:A:2068:THR:HG23	2.19	0.42
1:A:2462:TYR:CZ	1:A:2464:GLY:HA3	2.54	0.42
1:B:578:ALA:HA	1:B:628:THR:HG23	2.01	0.42
1:B:1446:VAL:HG13	1:B:1448:ASN:H	1.84	0.42
1:B:2032:SER:C	1:B:2033:MET:HE2	2.43	0.42
1:B:2097:LEU:HD21	1:C:2267:HIS:HE1	1.83	0.42
1:B:2462:TYR:CZ	1:B:2464:GLY:HA3	2.54	0.42
1:C:489:THR:HA	1:C:503:ALA:HB1	2.01	0.42
1:C:1733:GLN:C	1:C:1735:ILE:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1745:PHE:HB3	1:C:1758:ILE:HD12	2.01	0.42
1:C:1895:ASP:O	1:C:1899:LEU:HD23	2.18	0.42
1:C:2158:GLN:NE2	1:D:2199:MET:HB2	2.29	0.42
1:D:680:LEU:HD23	1:D:744:VAL:HG13	2.01	0.42
1:D:1181:THR:OG1	1:D:1184:LYS:HB2	2.18	0.42
1:D:1651:ARG:HA	1:D:1856:ARG:HH11	1.85	0.42
1:E:687:ILE:HG13	1:E:691:MET:SD	2.58	0.42
1:E:1417:VAL:HG12	1:E:1426:ALA:HB3	2.00	0.42
1:E:2032:SER:C	1:E:2033:MET:HE2	2.43	0.42
1:E:2198:VAL:HA	1:E:2201:LEU:HG	2.00	0.42
1:A:1520:THR:OG1	1:A:1573:VAL:HB	2.19	0.42
1:A:1875:ASP:O	1:A:1879:GLN:HG3	2.20	0.42
1:B:26:GLN:HA	1:B:57:LYS:HZ1	1.82	0.42
1:B:642:TRP:O	1:B:645:GLN:HG2	2.19	0.42
1:C:1214:ILE:O	1:C:1218:VAL:HG23	2.19	0.42
1:C:2061:ARG:HG3	1:C:2348:LEU:HD13	2.01	0.42
1:C:2375:TYR:CD2	1:C:2385:LEU:HD13	2.54	0.42
1:D:732:PRO:HB3	1:D:763:VAL:HG21	2.00	0.42
1:D:1520:THR:OG1	1:D:1573:VAL:HB	2.19	0.42
1:D:2093:GLN:HA	1:D:2096:GLU:CD	2.45	0.42
1:D:2217:GLU:O	1:D:2221:ARG:HG2	2.20	0.42
1:D:2375:TYR:CD2	1:D:2385:LEU:HD13	2.54	0.42
1:E:589:LEU:HD23	1:E:589:LEU:HA	1.88	0.42
1:E:1757:LEU:HD22	1:E:1760:ASP:HB3	2.01	0.42
1:E:2119:LEU:HD12	1:E:2119:LEU:HA	1.79	0.42
1:A:578:ALA:HA	1:A:628:THR:HG23	2.02	0.42
1:A:680:LEU:HD23	1:A:744:VAL:HG13	2.01	0.42
1:A:732:PRO:HB3	1:A:763:VAL:HG21	2.00	0.42
1:A:750:ASN:HB3	1:A:753:GLU:HB2	2.00	0.42
1:A:1476:THR:O	1:A:1480:LYS:HG2	2.19	0.42
1:B:1214:ILE:O	1:B:1218:VAL:HG23	2.19	0.42
1:B:1494:PHE:CE2	1:B:1496:ILE:HG12	2.54	0.42
1:C:901:ALA:O	1:C:902:LEU:HG	2.20	0.42
1:C:1446:VAL:HG13	1:C:1448:ASN:H	1.84	0.42
1:C:1454:LEU:HD12	1:C:1482:CYS:SG	2.59	0.42
1:C:1459:PHE:HB3	1:C:1461:PRO:O	2.19	0.42
1:D:687:ILE:HG13	1:D:691:MET:SD	2.58	0.42
1:D:1255:TYR:CE2	1:D:1296:ILE:HG22	2.52	0.42
1:D:1393:GLY:HA2	1:D:1511:GLY:HA2	2.01	0.42
1:D:2064:VAL:O	1:D:2068:THR:HG23	2.19	0.42
1:E:91:SER:O	1:E:94:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2061:ARG:HG3	1:E:2348:LEU:HD13	2.01	0.42
1:A:450:LYS:HD3	1:A:478:ILE:HD12	2.01	0.42
1:A:468:ILE:HD13	1:A:486:VAL:HG22	2.02	0.42
1:A:737:ILE:HG22	1:A:741:MET:HE1	2.00	0.42
1:A:1122:TRP:CE2	1:A:1144:THR:HB	2.54	0.42
1:A:1162:PHE:CD2	1:A:1163:ARG:HG2	2.54	0.42
1:A:1393:GLY:HA2	1:A:1511:GLY:HA2	2.01	0.42
1:A:1895:ASP:O	1:A:1899:LEU:HD23	2.18	0.42
1:A:2061:ARG:HG3	1:A:2348:LEU:HD13	2.01	0.42
1:A:2217:GLU:O	1:A:2221:ARG:HG2	2.19	0.42
1:B:901:ALA:O	1:B:902:LEU:HG	2.20	0.42
1:B:1757:LEU:HD22	1:B:1760:ASP:HB3	2.00	0.42
1:C:642:TRP:O	1:C:645:GLN:HG2	2.19	0.42
1:C:1162:PHE:HE2	1:C:1272:GLY:HA2	1.84	0.42
1:C:1417:VAL:HG12	1:C:1426:ALA:HB3	2.00	0.42
1:C:1651:ARG:HA	1:C:1856:ARG:HH11	1.84	0.42
1:C:2300:PHE:CE2	1:C:2331:TRP:HB2	2.54	0.42
1:D:119:LEU:HB2	1:D:990:ILE:HD11	2.00	0.42
1:D:696:ASN:HB3	1:D:699:LEU:HB3	2.02	0.42
1:D:901:ALA:O	1:D:902:LEU:HG	2.20	0.42
1:E:901:ALA:O	1:E:902:LEU:HG	2.20	0.42
1:E:1446:VAL:HG13	1:E:1448:ASN:H	1.84	0.42
1:E:1453:ARG:NE	1:E:1456:GLU:HB2	2.33	0.42
1:E:1733:GLN:C	1:E:1735:ILE:H	2.26	0.42
1:A:1217:GLN:HG2	1:A:1278:LYS:NZ	2.35	0.42
1:A:1446:VAL:HG13	1:A:1448:ASN:H	1.84	0.42
1:A:1608:GLU:HB2	1:A:1614:GLN:HG2	2.01	0.42
1:B:1163:ARG:C	1:B:1164:GLU:HG3	2.44	0.42
1:B:1520:THR:OG1	1:B:1573:VAL:HB	2.19	0.42
1:B:2093:GLN:HA	1:B:2096:GLU:CD	2.45	0.42
1:C:737:ILE:HG22	1:C:741:MET:HE1	2.00	0.42
1:C:1163:ARG:C	1:C:1164:GLU:HG3	2.44	0.42
1:C:1494:PHE:CE2	1:C:1496:ILE:HG12	2.54	0.42
1:C:1757:LEU:HD22	1:C:1760:ASP:HB3	2.01	0.42
1:C:2217:GLU:O	1:C:2221:ARG:HG2	2.20	0.42
1:C:2392:PHE:CD1	1:C:2398:GLY:HA3	2.54	0.42
1:D:1494:PHE:CE2	1:D:1496:ILE:HG12	2.54	0.42
1:D:1930:GLU:HB3	1:D:1994:TRP:CE2	2.54	0.42
1:D:2364:GLU:HG3	1:D:2538:THR:HG22	2.01	0.42
1:E:708:ILE:HA	1:E:711:THR:HG22	2.00	0.42
1:E:1122:TRP:CE2	1:E:1144:THR:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1651:ARG:HA	1:E:1856:ARG:HH11	1.85	0.42
1:A:573:GLN:HA	1:A:576:LYS:HE2	2.02	0.42
1:A:901:ALA:O	1:A:902:LEU:HG	2.20	0.42
1:A:1459:PHE:HB3	1:A:1461:PRO:O	2.19	0.42
1:A:1494:PHE:CE2	1:A:1496:ILE:HG12	2.54	0.42
1:A:1960:LEU:HD23	1:A:1960:LEU:HA	1.88	0.42
1:B:737:ILE:HG22	1:B:741:MET:HE1	2.00	0.42
1:B:1217:GLN:HG2	1:B:1278:LYS:NZ	2.35	0.42
1:B:1651:ARG:HA	1:B:1856:ARG:HH11	1.84	0.42
1:B:1875:ASP:O	1:B:1879:GLN:HG3	2.20	0.42
1:B:2229:GLN:HE21	1:B:2229:GLN:HB2	1.73	0.42
1:B:2392:PHE:CD1	1:B:2398:GLY:HA3	2.54	0.42
1:C:468:ILE:HD13	1:C:486:VAL:HG22	2.02	0.42
1:D:127:LYS:HB3	1:D:127:LYS:HE2	1.85	0.42
1:D:750:ASN:HB3	1:D:753:GLU:HB2	2.00	0.42
1:D:1162:PHE:HE2	1:D:1272:GLY:HA2	1.85	0.42
1:D:1417:VAL:HG12	1:D:1426:ALA:HB3	2.00	0.42
1:D:1892:ARG:HD3	1:D:1892:ARG:HA	1.69	0.42
1:D:1960:LEU:HD23	1:D:1960:LEU:HA	1.88	0.42
1:D:2119:LEU:HG	1:D:2240:MET:HE2	2.02	0.42
1:D:2439:LEU:HG	1:D:2504:VAL:HA	2.02	0.42
1:E:172:HIS:CE1	1:E:175:ARG:HH21	2.38	0.42
1:E:754:THR:O	1:E:758:VAL:HG13	2.20	0.42
1:E:1218:VAL:HA	1:E:1221:VAL:HG22	2.02	0.42
1:E:1573:VAL:HA	1:E:1587:ILE:O	2.20	0.42
1:E:2342:GLU:HG2	1:E:2343:THR:N	2.35	0.42
1:A:30:PHE:HA	1:A:50:TYR:CE2	2.55	0.42
1:A:696:ASN:HB3	1:A:699:LEU:HB3	2.02	0.42
1:A:2236:GLU:HA	1:A:2239:GLN:HG2	2.02	0.42
1:B:573:GLN:HA	1:B:576:LYS:HE2	2.02	0.42
1:B:754:THR:O	1:B:758:VAL:HG13	2.20	0.42
1:B:1930:GLU:HB3	1:B:1994:TRP:CE2	2.54	0.42
1:B:2064:VAL:O	1:B:2068:THR:HG23	2.19	0.42
1:B:2236:GLU:HA	1:B:2239:GLN:HG2	2.02	0.42
1:D:91:SER:O	1:D:94:GLU:HG2	2.19	0.42
1:E:450:LYS:HD3	1:E:478:ILE:HD12	2.01	0.42
1:E:468:ILE:HD13	1:E:486:VAL:HG22	2.02	0.42
1:E:719:MET:SD	1:E:781:LEU:HD23	2.60	0.42
1:E:732:PRO:HB3	1:E:763:VAL:HG21	2.00	0.42
1:E:930:GLN:O	1:E:934:LEU:HD23	2.19	0.42
1:E:1243:THR:C	1:E:1244:LEU:HD22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1875:ASP:O	1:E:1879:GLN:HG3	2.20	0.42
1:E:2462:TYR:CZ	1:E:2464:GLY:HA3	2.54	0.42
1:A:754:THR:O	1:A:758:VAL:HG13	2.20	0.42
1:A:1485:ALA:O	1:A:1499:SER:HA	2.20	0.42
1:A:1757:LEU:HD22	1:A:1760:ASP:HB3	2.01	0.42
1:A:1892:ARG:HD3	1:A:1892:ARG:HA	1.69	0.42
1:A:1937:GLN:HE21	1:B:290:LEU:HD21	1.85	0.42
1:B:26:GLN:N	1:B:27:TYR:HB2	2.35	0.42
1:B:867:TRP:HA	1:B:870:ILE:HB	2.02	0.42
1:B:1162:PHE:CD2	1:B:1163:ARG:HG2	2.54	0.42
1:B:1243:THR:C	1:B:1244:LEU:HD22	2.45	0.42
1:B:2066:GLN:HA	1:B:2069:GLN:NE2	2.35	0.42
1:B:2204:THR:HG22	1:B:2208:TYR:CZ	2.55	0.42
1:C:30:PHE:HA	1:C:50:TYR:HE2	1.85	0.42
1:C:336:LYS:HB2	1:C:431:GLY:H	1.85	0.42
1:C:578:ALA:HA	1:C:628:THR:HG23	2.01	0.42
1:C:680:LEU:HD23	1:C:744:VAL:HG13	2.01	0.42
1:C:1875:ASP:O	1:C:1879:GLN:HG3	2.20	0.42
1:C:2346:LEU:HD21	1:D:2298:GLN:NE2	2.34	0.42
1:D:336:LYS:HB2	1:D:431:GLY:H	1.85	0.42
1:D:1218:VAL:HA	1:D:1221:VAL:HG22	2.02	0.42
1:D:1459:PHE:HB3	1:D:1461:PRO:O	2.19	0.42
1:D:1608:GLU:HB2	1:D:1614:GLN:HG2	2.01	0.42
1:D:1807:GLU:HA	1:D:1811:TYR:HD2	1.85	0.42
1:D:2462:TYR:CZ	1:D:2464:GLY:HA3	2.54	0.42
1:E:1162:PHE:HE2	1:E:1272:GLY:HA2	1.84	0.42
1:E:1217:GLN:HG2	1:E:1278:LYS:NZ	2.35	0.42
1:E:1485:ALA:O	1:E:1499:SER:HA	2.20	0.42
1:E:1520:THR:OG1	1:E:1573:VAL:HB	2.19	0.42
1:E:1930:GLU:HB3	1:E:1994:TRP:CE2	2.54	0.42
1:A:91:SER:O	1:A:94:GLU:HG2	2.20	0.42
1:A:1218:VAL:HA	1:A:1221:VAL:HG22	2.02	0.42
1:A:1454:LEU:HD12	1:A:1482:CYS:SG	2.59	0.42
1:A:2093:GLN:HA	1:A:2096:GLU:CD	2.45	0.42
1:A:2119:LEU:HD22	1:A:2247:LEU:HD12	2.01	0.42
1:A:2456:ILE:HG12	1:A:2524:LEU:HD21	2.01	0.42
1:B:30:PHE:HA	1:B:50:TYR:HE2	1.85	0.42
1:B:1459:PHE:HB3	1:B:1461:PRO:O	2.19	0.42
1:B:2119:LEU:HD22	1:B:2247:LEU:HD12	2.02	0.42
1:B:2198:VAL:HA	1:B:2201:LEU:HG	2.00	0.42
1:C:840:ARG:HD2	1:C:840:ARG:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1393:GLY:HA2	1:C:1511:GLY:HA2	2.01	0.42
1:C:1442:ILE:HA	1:C:1455:PHE:O	2.20	0.42
1:C:1476:THR:O	1:C:1480:LYS:HG2	2.19	0.42
1:C:1485:ALA:O	1:C:1499:SER:HA	2.20	0.42
1:C:1573:VAL:HA	1:C:1587:ILE:O	2.20	0.42
1:C:2119:LEU:HG	1:C:2240:MET:HE2	2.02	0.42
1:C:2439:LEU:HG	1:C:2504:VAL:HA	2.02	0.42
1:D:312:VAL:HG22	1:D:313:ASP:H	1.85	0.42
1:D:489:THR:HA	1:D:503:ALA:HB1	2.01	0.42
1:D:2066:GLN:HA	1:D:2069:GLN:NE2	2.35	0.42
1:D:2119:LEU:HD22	1:D:2247:LEU:HD12	2.01	0.42
1:E:1237:GLY:HA2	1:E:1244:LEU:HD13	2.02	0.42
1:E:1459:PHE:HB3	1:E:1461:PRO:O	2.19	0.42
1:E:1476:THR:O	1:E:1480:LYS:HG2	2.19	0.42
1:E:2066:GLN:HA	1:E:2069:GLN:NE2	2.35	0.42
1:E:2093:GLN:HA	1:E:2096:GLU:CD	2.45	0.42
1:E:2119:LEU:HG	1:E:2240:MET:HE2	2.02	0.42
1:A:172:HIS:CE1	1:A:175:ARG:HH21	2.38	0.42
1:A:1214:ILE:O	1:A:1218:VAL:HG23	2.19	0.42
1:A:2146:GLN:NE2	1:D:1067:LYS:HD2	2.35	0.42
1:B:468:ILE:HD13	1:B:486:VAL:HG22	2.02	0.42
1:B:696:ASN:HB3	1:B:699:LEU:HB3	2.02	0.42
1:B:732:PRO:HB3	1:B:763:VAL:HG21	2.00	0.42
1:B:1122:TRP:CE2	1:B:1144:THR:HB	2.54	0.42
1:B:1208:ALA:HB2	1:C:2164:VAL:HG22	2.02	0.42
1:B:1996:THR:O	1:B:1999:LEU:HG	2.20	0.42
1:C:142:ARG:HE	1:C:142:ARG:HB3	1.72	0.42
1:C:1217:GLN:HG2	1:C:1278:LYS:NZ	2.35	0.42
1:C:1608:GLU:HB2	1:C:1614:GLN:HG2	2.01	0.42
1:C:2064:VAL:O	1:C:2068:THR:HG23	2.19	0.42
1:C:2204:THR:HG22	1:C:2208:TYR:CZ	2.55	0.42
1:C:2229:GLN:HE21	1:C:2229:GLN:HB2	1.72	0.42
1:C:2236:GLU:HA	1:C:2239:GLN:CG	2.50	0.42
1:C:2236:GLU:HA	1:C:2239:GLN:HG2	2.02	0.42
1:C:2462:TYR:CZ	1:C:2464:GLY:HA3	2.54	0.42
1:D:1446:VAL:HG13	1:D:1449:ASN:H	1.85	0.42
1:D:1454:LEU:HD12	1:D:1482:CYS:SG	2.59	0.42
1:D:1937:GLN:HE21	1:E:290:LEU:HD11	1.85	0.42
1:D:2300:PHE:CE2	1:D:2331:TRP:HB2	2.54	0.42
1:E:578:ALA:HA	1:E:628:THR:HG23	2.02	0.42
1:A:719:MET:SD	1:A:781:LEU:HD23	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:CYS:HA	1:A:764:MET:HE2	2.02	0.41
1:A:867:TRP:HA	1:A:870:ILE:HB	2.02	0.41
1:A:995:LEU:O	1:A:999:ARG:HG3	2.20	0.41
1:A:1651:ARG:HA	1:A:1856:ARG:HH11	1.85	0.41
1:A:1996:THR:O	1:A:1999:LEU:HG	2.20	0.41
1:A:2066:GLN:HA	1:A:2069:GLN:NE2	2.35	0.41
1:A:2260:TYR:CE2	1:E:2097:LEU:HD22	2.54	0.41
1:B:336:LYS:HB2	1:B:431:GLY:H	1.85	0.41
1:B:680:LEU:HD23	1:B:744:VAL:HG13	2.01	0.41
1:B:719:MET:SD	1:B:781:LEU:HD23	2.60	0.41
1:B:1485:ALA:O	1:B:1499:SER:HA	2.20	0.41
1:B:1892:ARG:HD3	1:B:1892:ARG:HA	1.69	0.41
1:C:573:GLN:HA	1:C:576:LYS:HE2	2.02	0.41
1:C:2093:GLN:HA	1:C:2096:GLU:CD	2.45	0.41
1:C:2342:GLU:CG	1:D:2295:ILE:HD13	2.50	0.41
1:D:468:ILE:HD13	1:D:486:VAL:HG22	2.02	0.41
1:E:312:VAL:HG22	1:E:313:ASP:H	1.85	0.41
1:E:573:GLN:HA	1:E:576:LYS:HE2	2.02	0.41
1:E:1494:PHE:CE2	1:E:1496:ILE:HG12	2.54	0.41
1:E:2119:LEU:HD22	1:E:2247:LEU:HD12	2.01	0.41
1:A:26:GLN:N	1:A:27:TYR:HB2	2.35	0.41
1:A:127:LYS:HB3	1:A:127:LYS:HE2	1.85	0.41
1:A:642:TRP:O	1:A:645:GLN:HG2	2.19	0.41
1:A:684:ARG:HG2	1:A:745:LEU:HA	2.03	0.41
1:A:930:GLN:O	1:A:934:LEU:HD23	2.19	0.41
1:A:2364:GLU:HG3	1:A:2538:THR:HG22	2.01	0.41
1:B:1454:LEU:HD12	1:B:1482:CYS:SG	2.59	0.41
1:B:1807:GLU:HA	1:B:1811:TYR:HD2	1.85	0.41
1:B:2236:GLU:HA	1:B:2239:GLN:CG	2.50	0.41
1:B:2364:GLU:HG3	1:B:2538:THR:HG22	2.01	0.41
1:C:1243:THR:C	1:C:1244:LEU:HD22	2.45	0.41
1:C:2066:GLN:HA	1:C:2069:GLN:NE2	2.35	0.41
1:D:26:GLN:N	1:D:27:TYR:HB2	2.35	0.41
1:D:2061:ARG:HG3	1:D:2348:LEU:HD13	2.01	0.41
1:D:2092:GLN:O	1:D:2096:GLU:OE1	2.38	0.41
1:D:2204:THR:HG22	1:D:2208:TYR:CZ	2.55	0.41
1:D:2236:GLU:HA	1:D:2239:GLN:HG2	2.02	0.41
1:E:995:LEU:O	1:E:999:ARG:HG3	2.20	0.41
1:E:2236:GLU:HA	1:E:2239:GLN:HG2	2.02	0.41
1:E:2375:TYR:CD2	1:E:2385:LEU:HD13	2.54	0.41
1:E:2456:ILE:HG12	1:E:2524:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:THR:HA	1:A:503:ALA:HB1	2.01	0.41
1:A:1237:GLY:HA2	1:A:1244:LEU:HD13	2.02	0.41
1:A:2236:GLU:HA	1:A:2239:GLN:CG	2.50	0.41
1:B:1059:LEU:HD22	1:B:1080:TYR:CD1	2.55	0.41
1:B:2375:TYR:CD2	1:B:2385:LEU:HD13	2.54	0.41
1:C:2158:GLN:OE1	1:D:2203:ALA:HB2	2.20	0.41
1:D:578:ALA:HA	1:D:628:THR:HG23	2.02	0.41
1:D:642:TRP:O	1:D:645:GLN:HG2	2.19	0.41
1:D:737:ILE:HG22	1:D:741:MET:HE1	2.00	0.41
1:D:1996:THR:O	1:D:1999:LEU:HG	2.20	0.41
1:D:2456:ILE:HG12	1:D:2524:LEU:HD21	2.01	0.41
1:E:489:THR:HA	1:E:503:ALA:HB1	2.01	0.41
1:E:1393:GLY:HA2	1:E:1511:GLY:HA2	2.01	0.41
1:E:1446:VAL:HG13	1:E:1449:ASN:H	1.85	0.41
1:E:2240:MET:HE2	1:E:2240:MET:HB2	1.92	0.41
1:E:2439:LEU:HG	1:E:2504:VAL:HA	2.02	0.41
1:E:2537:TYR:HE2	1:E:2539:ILE:HD11	1.86	0.41
1:A:999:ARG:HG2	1:E:1925:GLU:OE2	2.21	0.41
1:A:1243:THR:C	1:A:1244:LEU:HD22	2.45	0.41
1:A:1930:GLU:HB3	1:A:1994:TRP:CE2	2.54	0.41
1:A:2342:GLU:HG2	1:A:2343:THR:N	2.35	0.41
1:B:439:TYR:CD1	1:B:443:ILE:HD12	2.55	0.41
1:B:1573:VAL:HA	1:B:1587:ILE:O	2.20	0.41
1:B:2217:GLU:O	1:B:2221:ARG:HG2	2.20	0.41
1:B:2439:LEU:HG	1:B:2504:VAL:HA	2.02	0.41
1:C:30:PHE:HA	1:C:50:TYR:CE2	2.55	0.41
1:C:696:ASN:HB3	1:C:699:LEU:HB3	2.02	0.41
1:C:1059:LEU:HD22	1:C:1080:TYR:CD1	2.55	0.41
1:C:1446:VAL:HG13	1:C:1449:ASN:H	1.85	0.41
1:D:589:LEU:HD23	1:D:589:LEU:HA	1.88	0.41
1:D:719:MET:SD	1:D:781:LEU:HD23	2.60	0.41
1:D:761:CYS:HA	1:D:764:MET:HG2	2.02	0.41
1:D:867:TRP:HA	1:D:870:ILE:HB	2.02	0.41
1:D:1875:ASP:O	1:D:1879:GLN:HG3	2.20	0.41
1:E:10:LYS:HB3	1:E:10:LYS:HE3	1.94	0.41
1:E:1442:ILE:HA	1:E:1455:PHE:O	2.20	0.41
1:E:1608:GLU:HB2	1:E:1614:GLN:HG2	2.01	0.41
1:E:1996:THR:O	1:E:1999:LEU:HG	2.20	0.41
1:A:312:VAL:HG22	1:A:313:ASP:H	1.85	0.41
1:A:336:LYS:HB2	1:A:431:GLY:H	1.85	0.41
1:A:1573:VAL:HA	1:A:1587:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2204:THR:HG22	1:A:2208:TYR:CZ	2.55	0.41
1:B:312:VAL:HG22	1:B:313:ASP:H	1.85	0.41
1:B:2195:SER:O	1:B:2199:MET:HG3	2.21	0.41
1:B:2475:ILE:HG23	1:B:2499:PHE:CE2	2.56	0.41
1:C:26:GLN:N	1:C:27:TYR:HB2	2.35	0.41
1:C:91:SER:O	1:C:94:GLU:HG2	2.19	0.41
1:C:719:MET:SD	1:C:781:LEU:HD23	2.60	0.41
1:C:1218:VAL:HA	1:C:1221:VAL:HG22	2.02	0.41
1:C:1237:GLY:HA2	1:C:1244:LEU:HD13	2.02	0.41
1:C:1996:THR:O	1:C:1999:LEU:HG	2.20	0.41
1:C:2339:MET:CE	1:D:2288:MET:SD	3.09	0.41
1:D:406:ASP:HA	1:D:409:TYR:HB3	2.03	0.41
1:D:414:LYS:HA	1:D:414:LYS:HD2	1.79	0.41
1:D:1237:GLY:HA2	1:D:1244:LEU:HD13	2.02	0.41
1:D:1476:THR:O	1:D:1480:LYS:HG2	2.19	0.41
1:D:2236:GLU:HA	1:D:2239:GLN:CG	2.50	0.41
1:E:30:PHE:HA	1:E:50:TYR:CE2	2.55	0.41
1:E:705:ALA:HB1	1:E:717:PRO:O	2.21	0.41
1:E:1046:PRO:HG2	1:E:1892:ARG:HE	1.86	0.41
1:E:1454:LEU:HD12	1:E:1482:CYS:SG	2.59	0.41
1:E:2064:VAL:O	1:E:2068:THR:HG23	2.19	0.41
1:E:2092:GLN:O	1:E:2096:GLU:OE1	2.38	0.41
1:E:2217:GLU:O	1:E:2221:ARG:HG2	2.19	0.41
1:B:30:PHE:HA	1:B:50:TYR:CE2	2.55	0.41
1:B:2233:ALA:O	1:B:2236:GLU:HG3	2.21	0.41
1:C:329:ALA:HB3	1:C:444:PHE:CE2	2.55	0.41
1:C:2119:LEU:HD22	1:C:2247:LEU:HD12	2.01	0.41
1:C:2233:ALA:O	1:C:2236:GLU:HG3	2.21	0.41
1:D:1217:GLN:HG2	1:D:1278:LYS:NZ	2.35	0.41
1:D:2491:PHE:HB2	1:E:2488:MET:HE1	2.01	0.41
1:D:2537:TYR:HE2	1:D:2539:ILE:HD11	1.86	0.41
1:E:329:ALA:HB3	1:E:444:PHE:CE2	2.55	0.41
1:E:642:TRP:O	1:E:645:GLN:HG2	2.19	0.41
1:E:840:ARG:HD2	1:E:840:ARG:HA	1.81	0.41
1:A:329:ALA:HB3	1:A:444:PHE:CE2	2.55	0.41
1:A:452:ILE:HD12	1:A:452:ILE:HA	1.96	0.41
1:A:1442:ILE:HA	1:A:1455:PHE:O	2.20	0.41
1:A:2097:LEU:HD21	1:B:2267:HIS:HE1	1.84	0.41
1:B:91:SER:O	1:B:94:GLU:HG2	2.20	0.41
1:B:660:ILE:HD12	1:B:660:ILE:HA	1.97	0.41
1:B:1446:VAL:HG13	1:B:1449:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2274:LEU:O	1:B:2278:LYS:HG2	2.21	0.41
1:C:312:VAL:HG22	1:C:313:ASP:H	1.85	0.41
1:C:705:ALA:HB1	1:C:717:PRO:O	2.21	0.41
1:C:1520:THR:OG1	1:C:1573:VAL:HB	2.19	0.41
1:C:2142:ASN:HD21	1:D:2217:GLU:CD	2.28	0.41
1:D:30:PHE:HA	1:D:50:TYR:HE2	1.85	0.41
1:D:504:GLN:HG2	1:D:509:SER:HB2	2.03	0.41
1:D:754:THR:O	1:D:758:VAL:HG13	2.20	0.41
1:D:1485:ALA:O	1:D:1499:SER:HA	2.20	0.41
1:E:26:GLN:N	1:E:27:TYR:HB2	2.35	0.41
1:E:867:TRP:HA	1:E:870:ILE:HB	2.02	0.41
1:E:2119:LEU:HA	1:E:2122:SER:HB2	2.02	0.41
1:E:2195:SER:O	1:E:2199:MET:HG3	2.21	0.41
1:A:30:PHE:HA	1:A:50:TYR:HE2	1.85	0.41
1:A:1059:LEU:HD22	1:A:1080:TYR:CD1	2.55	0.41
1:A:2475:ILE:HG23	1:A:2499:PHE:CE2	2.56	0.41
1:B:454:LEU:HD11	1:B:465:LEU:HD22	2.03	0.41
1:B:1162:PHE:HE2	1:B:1272:GLY:HA2	1.84	0.41
1:B:1218:VAL:HA	1:B:1221:VAL:HG22	2.02	0.41
1:B:1442:ILE:HA	1:B:1455:PHE:O	2.20	0.41
1:B:2061:ARG:HG3	1:B:2348:LEU:HD13	2.01	0.41
1:B:2119:LEU:HG	1:B:2240:MET:HE2	2.02	0.41
1:C:10:LYS:HB3	1:C:10:LYS:HE3	1.94	0.41
1:C:57:LYS:HA	1:C:57:LYS:HD3	1.92	0.41
1:C:1898:ILE:HD11	1:C:1997:LEU:HD21	2.02	0.41
1:C:2067:LEU:HG	1:C:2296:TYR:HE1	1.86	0.41
1:C:2092:GLN:O	1:C:2096:GLU:OE1	2.38	0.41
1:D:169:LEU:O	1:D:173:ILE:HG12	2.21	0.41
1:D:948:ASN:C	1:D:948:ASN:HD22	2.28	0.41
1:D:1059:LEU:HD22	1:D:1080:TYR:CD1	2.55	0.41
1:D:1243:THR:C	1:D:1244:LEU:HD22	2.45	0.41
1:D:1442:ILE:HA	1:D:1455:PHE:O	2.20	0.41
1:D:1573:VAL:HA	1:D:1587:ILE:O	2.20	0.41
1:D:2119:LEU:HA	1:D:2122:SER:HB2	2.02	0.41
1:D:2233:ALA:O	1:D:2236:GLU:HG3	2.21	0.41
1:E:696:ASN:HB3	1:E:699:LEU:HB3	2.02	0.41
1:E:761:CYS:HA	1:E:764:MET:HG2	2.02	0.41
1:E:1577:LYS:HZ3	1:E:1581:GLY:HA2	1.84	0.41
1:E:2460:LEU:O	1:E:2474:ALA:HA	2.20	0.41
1:A:1004:ILE:HD13	1:E:1925:GLU:HG2	2.03	0.41
1:A:1425:ILE:HD13	1:A:1425:ILE:HA	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2119:LEU:HG	1:A:2240:MET:HE2	2.02	0.41
1:A:2274:LEU:O	1:A:2278:LYS:HG2	2.21	0.41
1:A:2537:TYR:HE2	1:A:2539:ILE:HD11	1.86	0.41
1:B:342:LYS:HD3	1:B:346:TYR:HA	2.03	0.41
1:B:1167:HIS:CE1	1:B:1199:PHE:HB3	2.56	0.41
1:B:1393:GLY:HA2	1:B:1511:GLY:HA2	2.01	0.41
1:B:2119:LEU:HA	1:B:2122:SER:HB2	2.02	0.41
1:B:2342:GLU:HG2	1:B:2343:THR:N	2.35	0.41
1:B:2460:LEU:O	1:B:2474:ALA:HA	2.20	0.41
1:C:169:LEU:O	1:C:173:ILE:HG12	2.21	0.41
1:C:172:HIS:CE1	1:C:175:ARG:HH21	2.38	0.41
1:C:321:VAL:HG11	1:C:324:GLU:HB3	2.03	0.41
1:C:406:ASP:HA	1:C:409:TYR:HB3	2.03	0.41
1:C:414:LYS:HA	1:C:414:LYS:HD2	1.80	0.41
1:C:665:THR:HA	1:C:666:PRO:HD3	1.93	0.41
1:C:761:CYS:HA	1:C:764:MET:HG2	2.02	0.41
1:C:1167:HIS:CE1	1:C:1199:PHE:HB3	2.56	0.41
1:C:1425:ILE:HD13	1:C:1425:ILE:HA	1.98	0.41
1:C:1647:MET:HE3	1:C:1854:ASN:C	2.46	0.41
1:C:2057:LEU:HD12	1:C:2348:LEU:HD22	2.03	0.41
1:C:2119:LEU:HA	1:C:2122:SER:HB2	2.02	0.41
1:C:2119:LEU:HA	1:C:2119:LEU:HD12	1.79	0.41
1:C:2122:SER:CB	1:D:2239:GLN:HE22	2.32	0.41
1:C:2342:GLU:HG2	1:C:2343:THR:N	2.35	0.41
1:C:2537:TYR:HE2	1:C:2539:ILE:HD11	1.86	0.41
1:D:573:GLN:HA	1:D:576:LYS:HE2	2.02	0.41
1:D:684:ARG:HG2	1:D:745:LEU:HA	2.03	0.41
1:D:2128:ASN:HA	1:D:2131:GLU:CD	2.46	0.41
1:D:2460:LEU:O	1:D:2474:ALA:HA	2.21	0.41
1:E:30:PHE:HA	1:E:50:TYR:HE2	1.85	0.41
1:E:336:LYS:HB2	1:E:431:GLY:H	1.85	0.41
1:E:342:LYS:HD3	1:E:346:TYR:HA	2.03	0.41
1:E:1059:LEU:HD22	1:E:1080:TYR:CD1	2.56	0.41
1:E:1298:HIS:HB3	1:E:1303:ASP:HB3	2.03	0.41
1:E:1647:MET:HE3	1:E:1854:ASN:C	2.46	0.41
1:E:2233:ALA:O	1:E:2236:GLU:HG3	2.21	0.41
1:A:1298:HIS:HB3	1:A:1303:ASP:HB3	2.03	0.41
1:A:1446:VAL:HG13	1:A:1449:ASN:H	1.85	0.41
1:A:1898:ILE:HD11	1:A:1997:LEU:HD21	2.03	0.41
1:A:2195:SER:O	1:A:2199:MET:HG3	2.21	0.41
1:B:172:HIS:CE1	1:B:175:ARG:HH21	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASP:HA	1:B:409:TYR:HB3	2.03	0.41
1:B:995:LEU:O	1:B:999:ARG:HG3	2.20	0.41
1:B:1066:SER:HB2	1:D:2141:ILE:HD12	2.01	0.41
1:B:2128:ASN:HA	1:B:2131:GLU:CD	2.46	0.41
1:C:504:GLN:HG2	1:C:509:SER:HB2	2.03	0.41
1:C:657:THR:O	1:C:660:ILE:HG22	2.21	0.41
1:C:1065:GLN:HG3	1:E:2212:LYS:NZ	2.35	0.41
1:D:30:PHE:HA	1:D:50:TYR:CE2	2.55	0.41
1:D:454:LEU:HD11	1:D:465:LEU:HD22	2.03	0.41
1:D:1167:HIS:CE1	1:D:1199:PHE:HB3	2.56	0.41
1:E:321:VAL:HG11	1:E:324:GLU:HB3	2.03	0.41
1:A:1665:PHE:HD2	1:A:1785:VAL:HG22	1.87	0.40
1:A:2057:LEU:HD12	1:A:2348:LEU:HD22	2.03	0.40
1:B:57:LYS:HA	1:B:57:LYS:HD3	1.92	0.40
1:B:657:THR:O	1:B:660:ILE:HG22	2.21	0.40
1:B:705:ALA:HB1	1:B:717:PRO:O	2.21	0.40
1:B:2092:GLN:O	1:B:2096:GLU:OE1	2.38	0.40
1:C:867:TRP:HA	1:C:870:ILE:HB	2.02	0.40
1:C:948:ASN:C	1:C:948:ASN:HD22	2.28	0.40
1:C:1648:GLU:HA	1:C:1651:ARG:HG2	2.03	0.40
1:C:1665:PHE:HD2	1:C:1785:VAL:HG22	1.87	0.40
1:D:329:ALA:HB3	1:D:444:PHE:CE2	2.56	0.40
1:D:657:THR:O	1:D:660:ILE:HG22	2.21	0.40
1:D:995:LEU:O	1:D:999:ARG:HG3	2.20	0.40
1:D:2475:ILE:HG23	1:D:2499:PHE:CE2	2.56	0.40
1:E:169:LEU:O	1:E:173:ILE:HG12	2.21	0.40
1:E:321:VAL:HG22	1:E:322:ASN:H	1.87	0.40
1:E:657:THR:O	1:E:660:ILE:HG22	2.21	0.40
1:E:948:ASN:C	1:E:948:ASN:HD22	2.28	0.40
1:E:1541:ALA:O	1:E:1547:MET:HE2	2.21	0.40
1:E:2204:THR:HG22	1:E:2208:TYR:CZ	2.55	0.40
1:E:2274:LEU:O	1:E:2278:LYS:HG2	2.21	0.40
1:A:1807:GLU:HA	1:A:1811:TYR:HD2	1.85	0.40
1:A:2092:GLN:O	1:A:2096:GLU:OE1	2.39	0.40
1:A:2233:ALA:O	1:A:2236:GLU:HG3	2.21	0.40
1:A:2437:ARG:CZ	1:A:2539:ILE:HD13	2.51	0.40
1:A:2439:LEU:HG	1:A:2504:VAL:HA	2.02	0.40
1:B:321:VAL:HG22	1:B:322:ASN:H	1.87	0.40
1:B:321:VAL:HG11	1:B:324:GLU:HB3	2.03	0.40
1:B:551:GLU:HG3	1:B:552:GLN:HG2	2.04	0.40
1:B:1046:PRO:HG2	1:B:1892:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1244:LEU:HB2	1:B:1270:ILE:CG2	2.51	0.40
1:B:1607:ARG:HE	1:B:1607:ARG:HB3	1.79	0.40
1:B:2537:TYR:HE2	1:B:2539:ILE:HD11	1.86	0.40
1:C:342:LYS:HD3	1:C:346:TYR:HA	2.03	0.40
1:C:754:THR:O	1:C:758:VAL:HG13	2.20	0.40
1:C:1244:LEU:HB2	1:C:1270:ILE:CG2	2.52	0.40
1:C:2065:ALA:O	1:C:2069:GLN:OE1	2.39	0.40
1:D:705:ALA:HB1	1:D:717:PRO:O	2.21	0.40
1:D:1741:TRP:CH2	1:D:1776:ILE:HG12	2.57	0.40
1:D:2057:LEU:HD12	1:D:2348:LEU:HD22	2.03	0.40
1:D:2067:LEU:HG	1:D:2296:TYR:HE1	1.86	0.40
1:D:2274:LEU:O	1:D:2278:LYS:HG2	2.21	0.40
1:E:1604:LEU:HA	1:E:1617:GLN:O	2.22	0.40
1:E:2065:ALA:O	1:E:2069:GLN:OE1	2.39	0.40
1:A:342:LYS:HD3	1:A:346:TYR:HA	2.03	0.40
1:A:660:ILE:HD12	1:A:660:ILE:HA	1.97	0.40
1:A:705:ALA:HB1	1:A:717:PRO:O	2.21	0.40
1:A:1167:HIS:CE1	1:A:1199:PHE:HB3	2.56	0.40
1:A:2460:LEU:O	1:A:2474:ALA:HA	2.20	0.40
1:B:169:LEU:O	1:B:173:ILE:HG12	2.21	0.40
1:B:2067:LEU:HG	1:B:2296:TYR:HE1	1.86	0.40
1:B:2146:GLN:HE21	1:E:1067:LYS:HD2	1.86	0.40
1:B:2292:LEU:O	1:B:2296:TYR:HB3	2.22	0.40
1:C:995:LEU:O	1:C:999:ARG:HG3	2.20	0.40
1:C:1541:ALA:O	1:C:1547:MET:HE2	2.21	0.40
1:C:2128:ASN:HA	1:C:2131:GLU:CD	2.46	0.40
1:C:2195:SER:O	1:C:2199:MET:HG3	2.21	0.40
1:C:2475:ILE:HG23	1:C:2499:PHE:CE2	2.56	0.40
1:D:342:LYS:HD3	1:D:346:TYR:HA	2.03	0.40
1:D:1046:PRO:HG2	1:D:1892:ARG:HE	1.86	0.40
1:D:1244:LEU:HB2	1:D:1270:ILE:CG2	2.52	0.40
1:D:1647:MET:HE3	1:D:1854:ASN:C	2.46	0.40
1:D:1665:PHE:HD2	1:D:1785:VAL:HG22	1.87	0.40
1:D:2065:ALA:O	1:D:2069:GLN:OE1	2.39	0.40
1:E:454:LEU:HD11	1:E:465:LEU:HD22	2.03	0.40
1:E:551:GLU:HG3	1:E:552:GLN:HG2	2.04	0.40
1:E:684:ARG:HG2	1:E:745:LEU:HA	2.02	0.40
1:E:704:LEU:HD11	1:E:741:MET:HE3	2.04	0.40
1:E:1244:LEU:HB2	1:E:1270:ILE:CG2	2.52	0.40
1:E:1461:PRO:HG2	1:E:1463:THR:O	2.22	0.40
1:E:1665:PHE:HD2	1:E:1785:VAL:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2236:GLU:HA	1:E:2239:GLN:CG	2.50	0.40
1:A:620:LEU:HD22	1:A:664:CYS:SG	2.62	0.40
1:A:704:LEU:HD11	1:A:741:MET:HE3	2.04	0.40
1:A:761:CYS:HA	1:A:764:MET:HG2	2.02	0.40
1:A:1647:MET:HE3	1:A:1854:ASN:C	2.46	0.40
1:A:1681:PHE:HD1	1:A:1702:LEU:HG	1.86	0.40
1:B:948:ASN:C	1:B:948:ASN:HD22	2.28	0.40
1:B:1237:GLY:HA2	1:B:1244:LEU:HD13	2.02	0.40
1:B:1461:PRO:HG2	1:B:1463:THR:O	2.22	0.40
1:C:439:TYR:CD1	1:C:443:ILE:HD12	2.55	0.40
1:C:761:CYS:HA	1:C:764:MET:HE2	2.02	0.40
1:C:897:ARG:HB2	1:C:908:ASN:HB2	2.03	0.40
1:C:1741:TRP:CH2	1:C:1776:ILE:HG12	2.56	0.40
1:C:1807:GLU:HA	1:C:1811:TYR:HD2	1.85	0.40
1:C:2245:GLU:O	1:C:2248:LYS:HG2	2.21	0.40
1:C:2274:LEU:O	1:C:2278:LYS:HG2	2.21	0.40
1:C:2437:ARG:CZ	1:C:2539:ILE:HD13	2.51	0.40
1:D:321:VAL:HG22	1:D:322:ASN:H	1.86	0.40
1:D:1604:LEU:HA	1:D:1617:GLN:O	2.22	0.40
1:D:1648:GLU:HA	1:D:1651:ARG:HG2	2.03	0.40
1:E:2067:LEU:HG	1:E:2296:TYR:HE1	1.86	0.40
1:A:169:LEU:O	1:A:173:ILE:HG12	2.21	0.40
1:A:321:VAL:HG11	1:A:324:GLU:HB3	2.03	0.40
1:A:657:THR:O	1:A:660:ILE:HG22	2.21	0.40
1:A:1244:LEU:HB2	1:A:1270:ILE:CG2	2.52	0.40
1:A:2119:LEU:HA	1:A:2122:SER:HB2	2.02	0.40
1:A:2128:ASN:HA	1:A:2131:GLU:CD	2.46	0.40
1:B:329:ALA:HB3	1:B:444:PHE:CE2	2.55	0.40
1:B:704:LEU:HD11	1:B:741:MET:HE3	2.04	0.40
1:C:1604:LEU:HA	1:C:1617:GLN:O	2.22	0.40
1:C:1814:MET:HE3	1:C:1814:MET:HB2	1.97	0.40
1:C:2460:LEU:O	1:C:2474:ALA:HA	2.20	0.40
1:D:321:VAL:HG11	1:D:324:GLU:HB3	2.03	0.40
1:D:704:LEU:HD11	1:D:741:MET:HE3	2.04	0.40
1:D:761:CYS:HA	1:D:764:MET:HE2	2.02	0.40
1:D:1541:ALA:O	1:D:1547:MET:HE2	2.21	0.40
1:D:2437:ARG:CZ	1:D:2539:ILE:HD13	2.51	0.40
1:E:504:GLN:HG2	1:E:509:SER:HB2	2.03	0.40
1:E:1807:GLU:HA	1:E:1811:TYR:HD2	1.85	0.40
1:E:2475:ILE:HG23	1:E:2499:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	43	77
1	B	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	43	77
1	C	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
1	D	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
1	E	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
All	All	12690/12700 (100%)	11872 (94%)	798 (6%)	20 (0%)	44	77

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2519	ASP
1	B	2519	ASP
1	C	2519	ASP
1	D	2519	ASP
1	E	2519	ASP
1	A	343	ASN
1	B	343	ASN
1	C	343	ASN
1	D	343	ASN
1	E	343	ASN
1	A	308	THR
1	B	308	THR
1	C	308	THR
1	D	308	THR
1	E	308	THR
1	A	2025	ASP
1	B	2025	ASP
1	C	2025	ASP
1	D	2025	ASP
1	E	2025	ASP

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	B	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	C	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	D	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	E	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
All	All	10875/10885 (100%)	10870 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2229	GLN
1	B	2229	GLN
1	C	2229	GLN
1	D	2229	GLN
1	E	2229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	193	GLN
1	A	266	ASN
1	A	294	GLN
1	A	345	ASN
1	A	362	ASN
1	A	449	ASN
1	A	750	ASN
1	A	801	GLN
1	A	802	HIS
1	A	953	ASN
1	A	1002	ASN
1	A	1314	GLN

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Mol	Chain	Res	Type
1	A	1638	ASN
1	A	1687	ASN
1	A	1733	GLN
1	A	1937	GLN
1	A	2261	GLN
1	A	2267	HIS
1	A	2298	GLN
1	A	2347	ASN
1	A	2391	GLN
1	A	2505	ASN
1	B	40	GLN
1	B	193	GLN
1	B	345	ASN
1	B	362	ASN
1	B	449	ASN
1	B	682	ASN
1	B	713	HIS
1	B	750	ASN
1	B	801	GLN
1	B	802	HIS
1	B	803	ASN
1	B	953	ASN
1	B	1002	ASN
1	B	1151	ASN
1	B	1314	GLN
1	B	1638	ASN
1	B	1687	ASN
1	B	1733	GLN
1	B	1937	GLN
1	B	2229	GLN
1	B	2261	GLN
1	B	2267	HIS
1	B	2298	GLN
1	B	2347	ASN
1	B	2479	HIS
1	B	2505	ASN
1	C	40	GLN
1	C	193	GLN
1	C	266	ASN
1	C	294	GLN
1	C	345	ASN
1	C	362	ASN

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Mol	Chain	Res	Type
1	C	449	ASN
1	C	750	ASN
1	C	801	GLN
1	C	802	HIS
1	C	953	ASN
1	C	1124	ASN
1	C	1314	GLN
1	C	1638	ASN
1	C	1687	ASN
1	C	1733	GLN
1	C	2229	GLN
1	C	2261	GLN
1	C	2267	HIS
1	C	2298	GLN
1	C	2347	ASN
1	C	2505	ASN
1	D	40	GLN
1	D	193	GLN
1	D	345	ASN
1	D	362	ASN
1	D	449	ASN
1	D	682	ASN
1	D	750	ASN
1	D	801	GLN
1	D	802	HIS
1	D	953	ASN
1	D	1151	ASN
1	D	1314	GLN
1	D	1404	HIS
1	D	1638	ASN
1	D	1687	ASN
1	D	1733	GLN
1	D	1937	GLN
1	D	2229	GLN
1	D	2261	GLN
1	D	2267	HIS
1	D	2298	GLN
1	D	2347	ASN
1	D	2391	GLN
1	D	2435	ASN
1	D	2505	ASN
1	E	40	GLN

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Mol	Chain	Res	Type
1	E	193	GLN
1	E	345	ASN
1	E	362	ASN
1	E	449	ASN
1	E	713	HIS
1	E	750	ASN
1	E	802	HIS
1	E	953	ASN
1	E	1002	ASN
1	E	1151	ASN
1	E	1314	GLN
1	E	1638	ASN
1	E	1687	ASN
1	E	1733	GLN
1	E	1937	GLN
1	E	2158	GLN
1	E	2229	GLN
1	E	2261	GLN
1	E	2267	HIS
1	E	2298	GLN
1	E	2347	ASN
1	E	2391	GLN
1	E	2413	GLN
1	E	2505	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

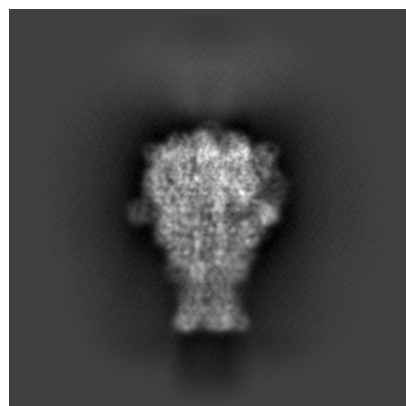
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48371. These allow visual inspection of the internal detail of the map and identification of artifacts.

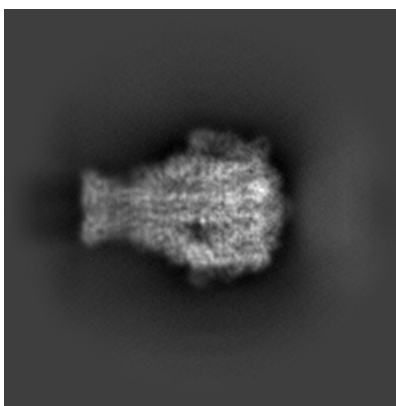
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

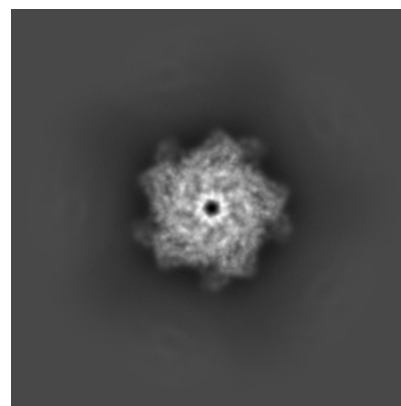
6.1.1 Primary map



X

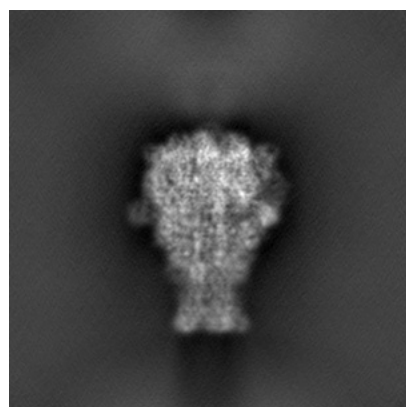


Y

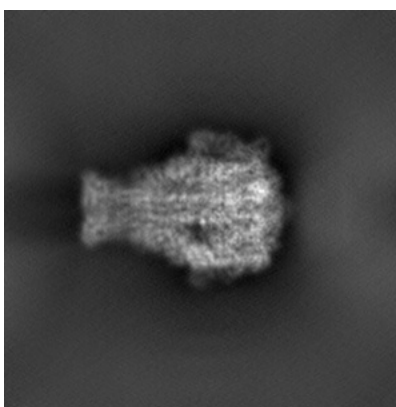


Z

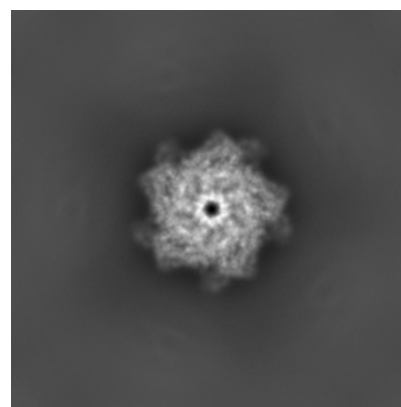
6.1.2 Raw map



X



Y

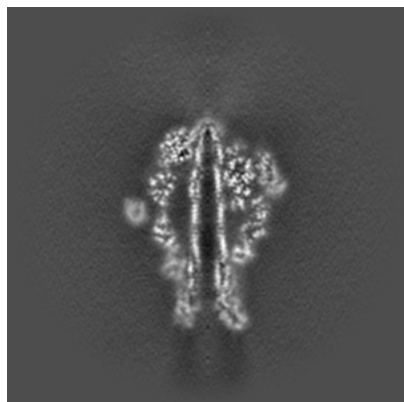


Z

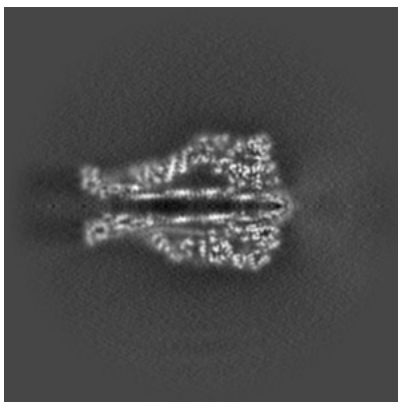
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

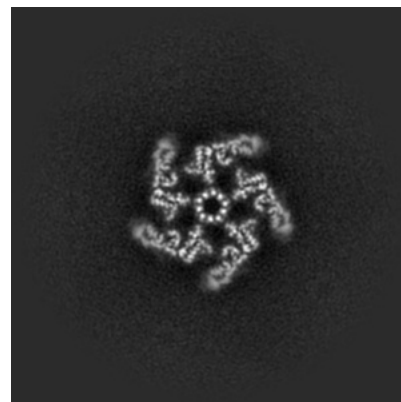
6.2.1 Primary map



X Index: 123

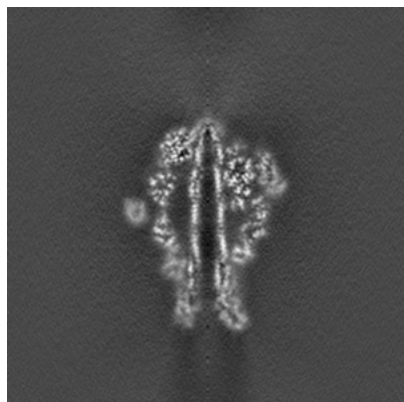


Y Index: 123

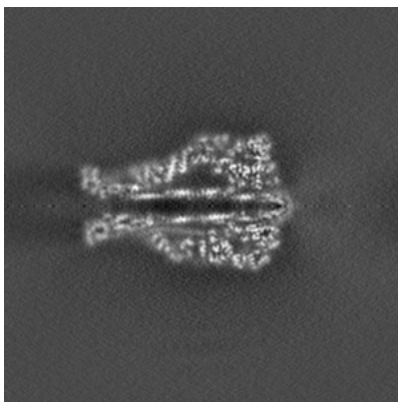


Z Index: 123

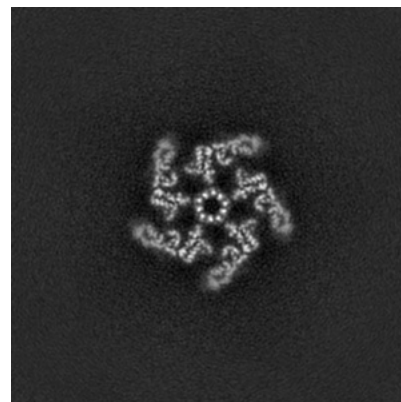
6.2.2 Raw map



X Index: 123



Y Index: 123

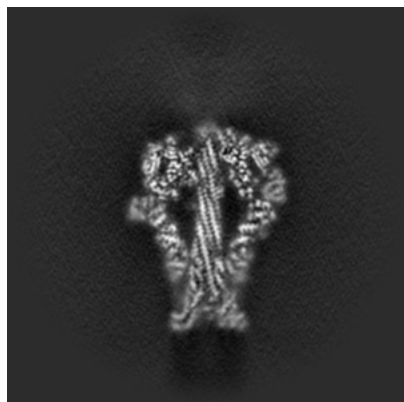


Z Index: 123

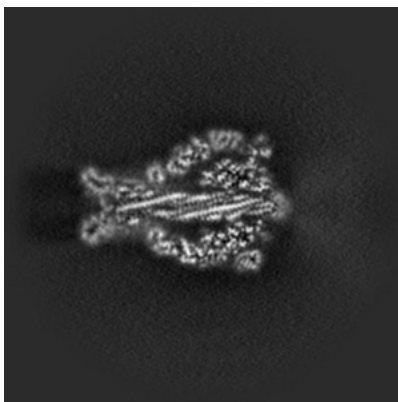
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

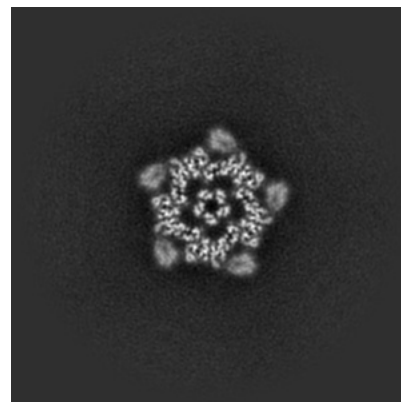
6.3.1 Primary map



X Index: 130

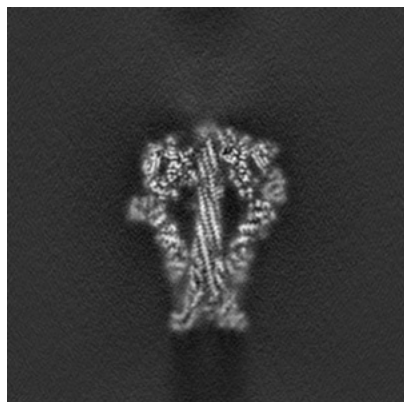


Y Index: 129

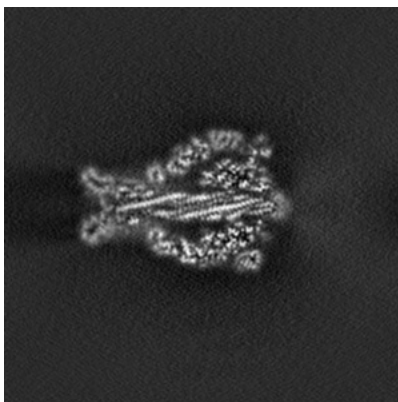


Z Index: 132

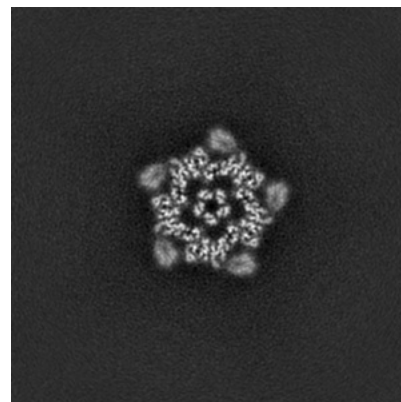
6.3.2 Raw map



X Index: 130



Y Index: 129

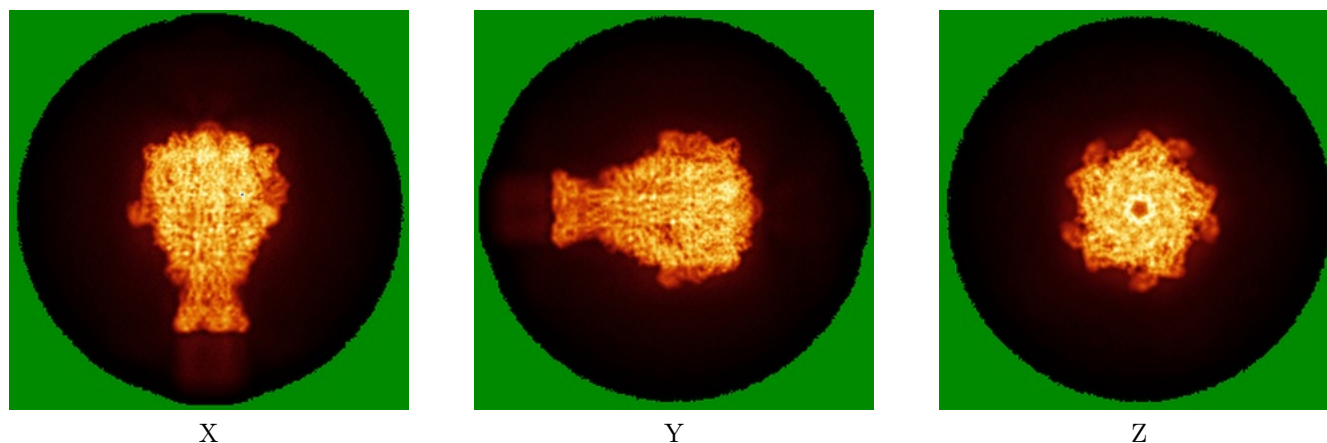


Z Index: 132

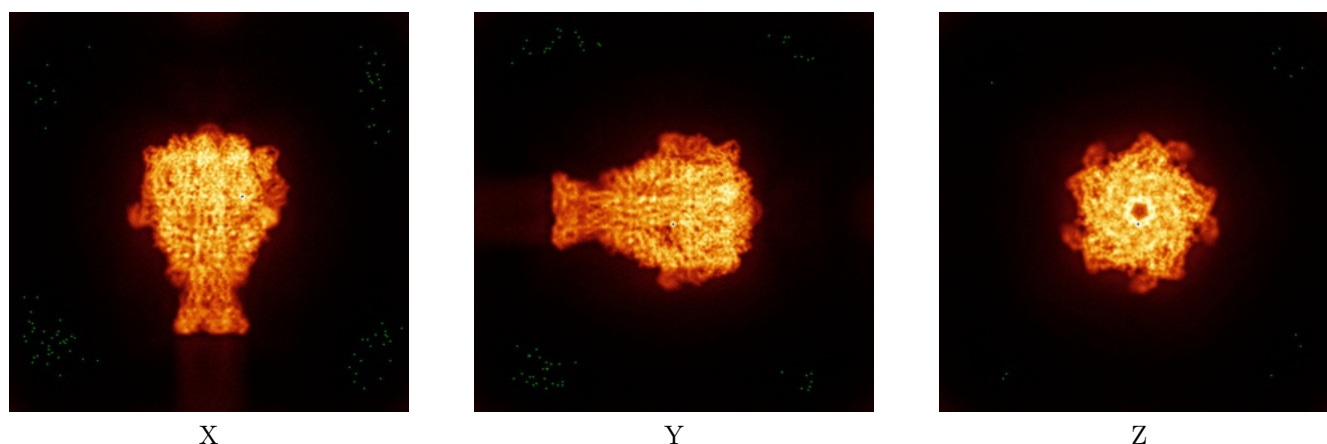
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

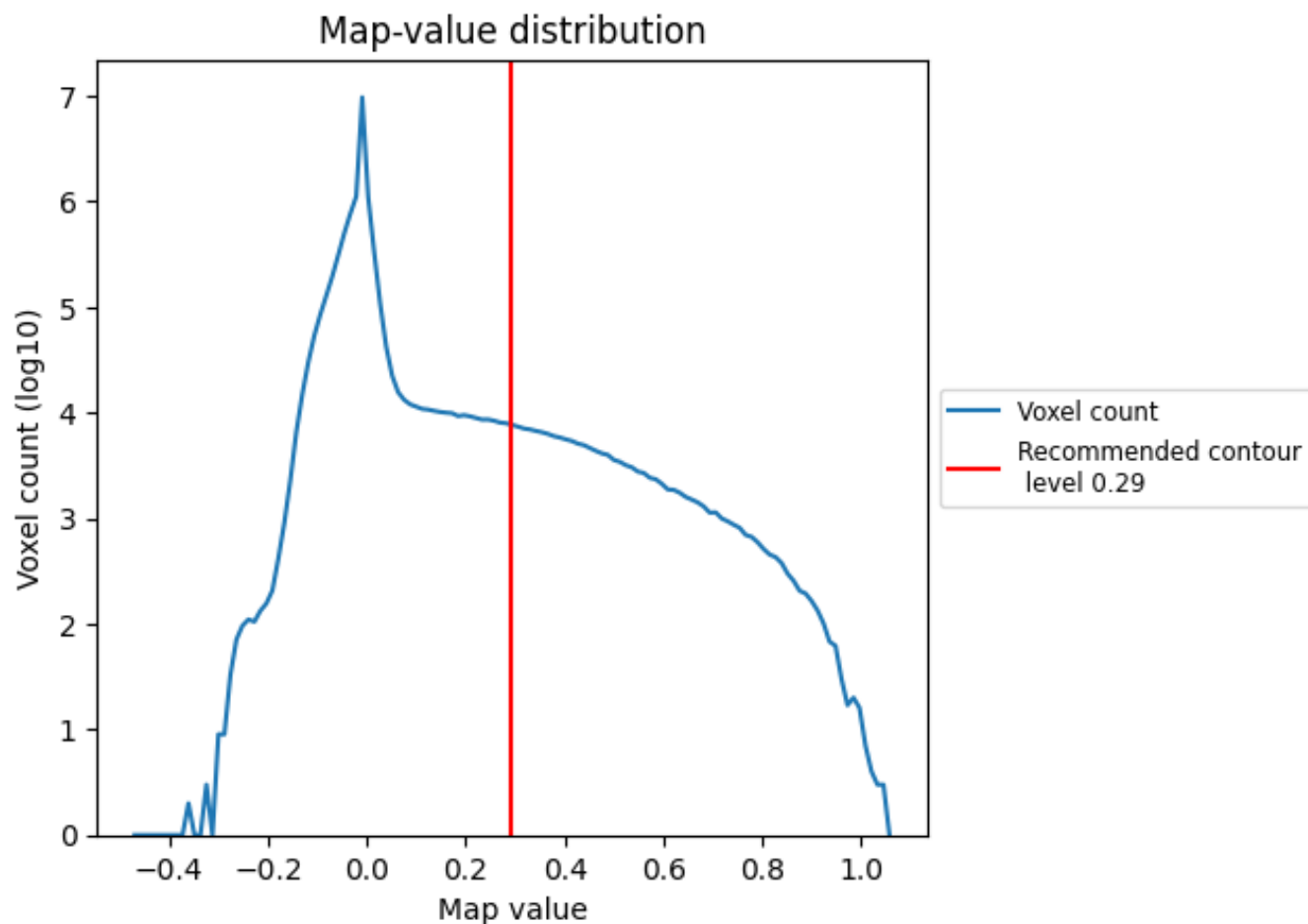
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

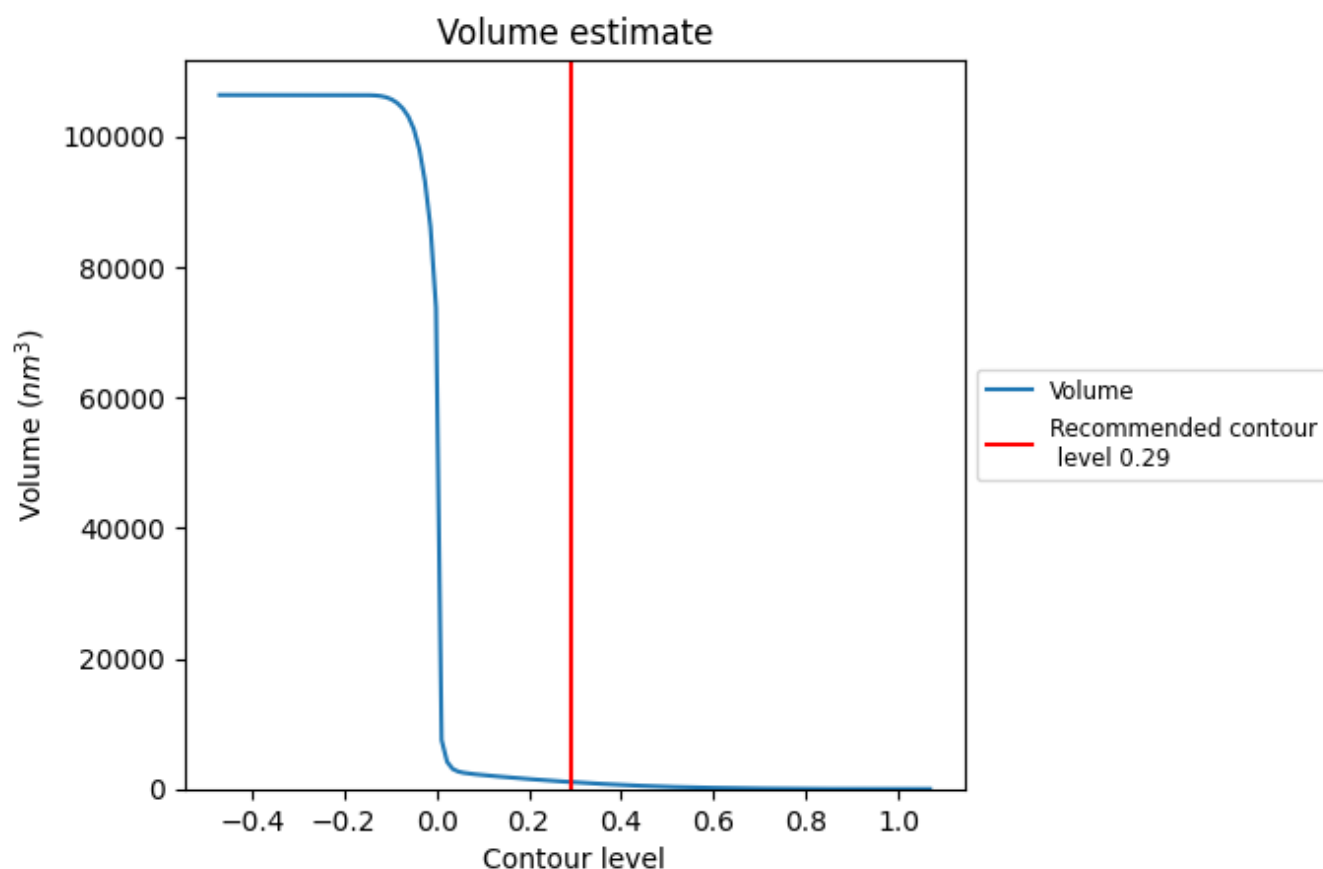
This section contains the results of statistical analysis of the map.

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.

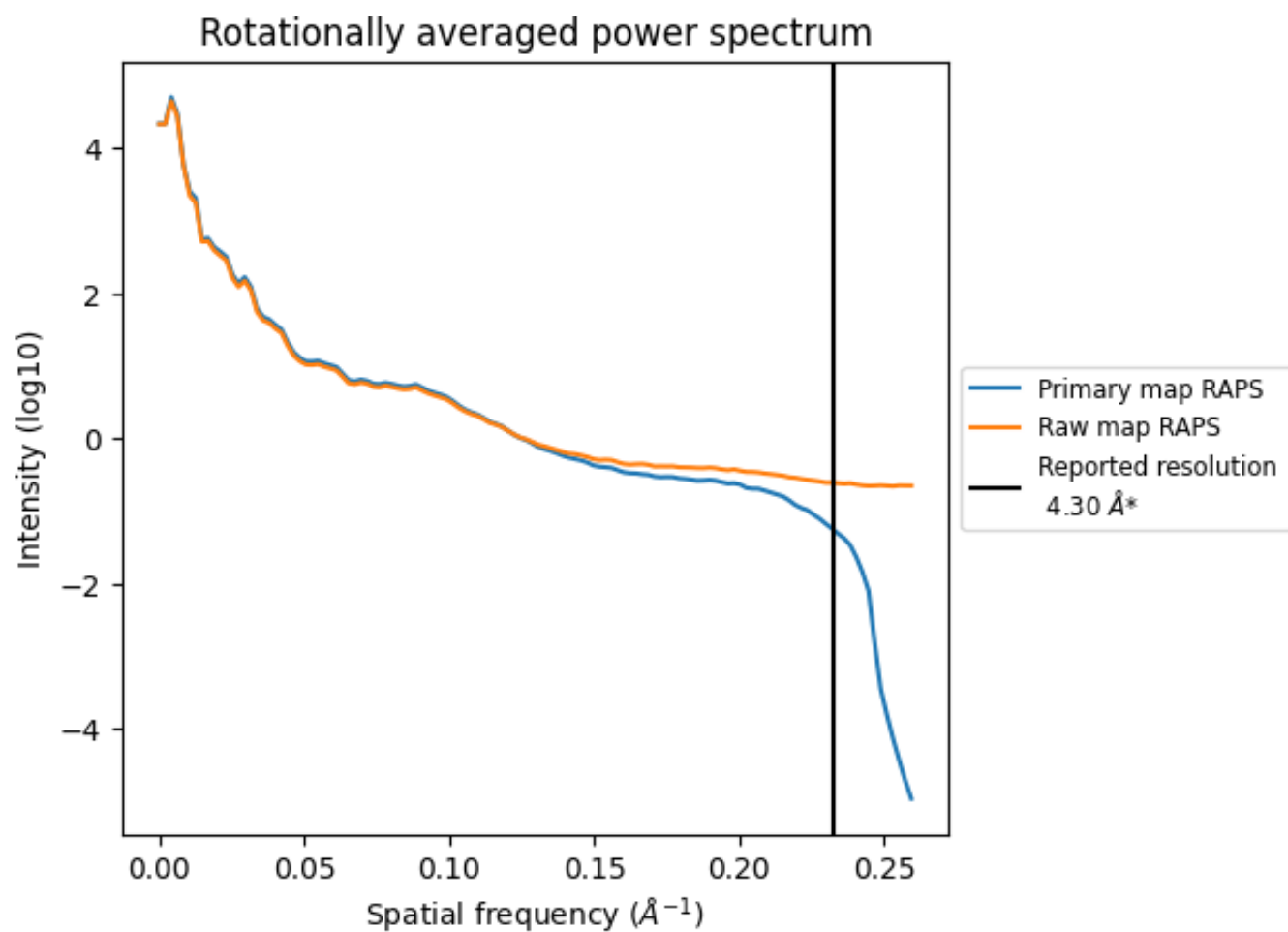
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1065 nm³; this corresponds to an approximate mass of 962 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 ⓘ

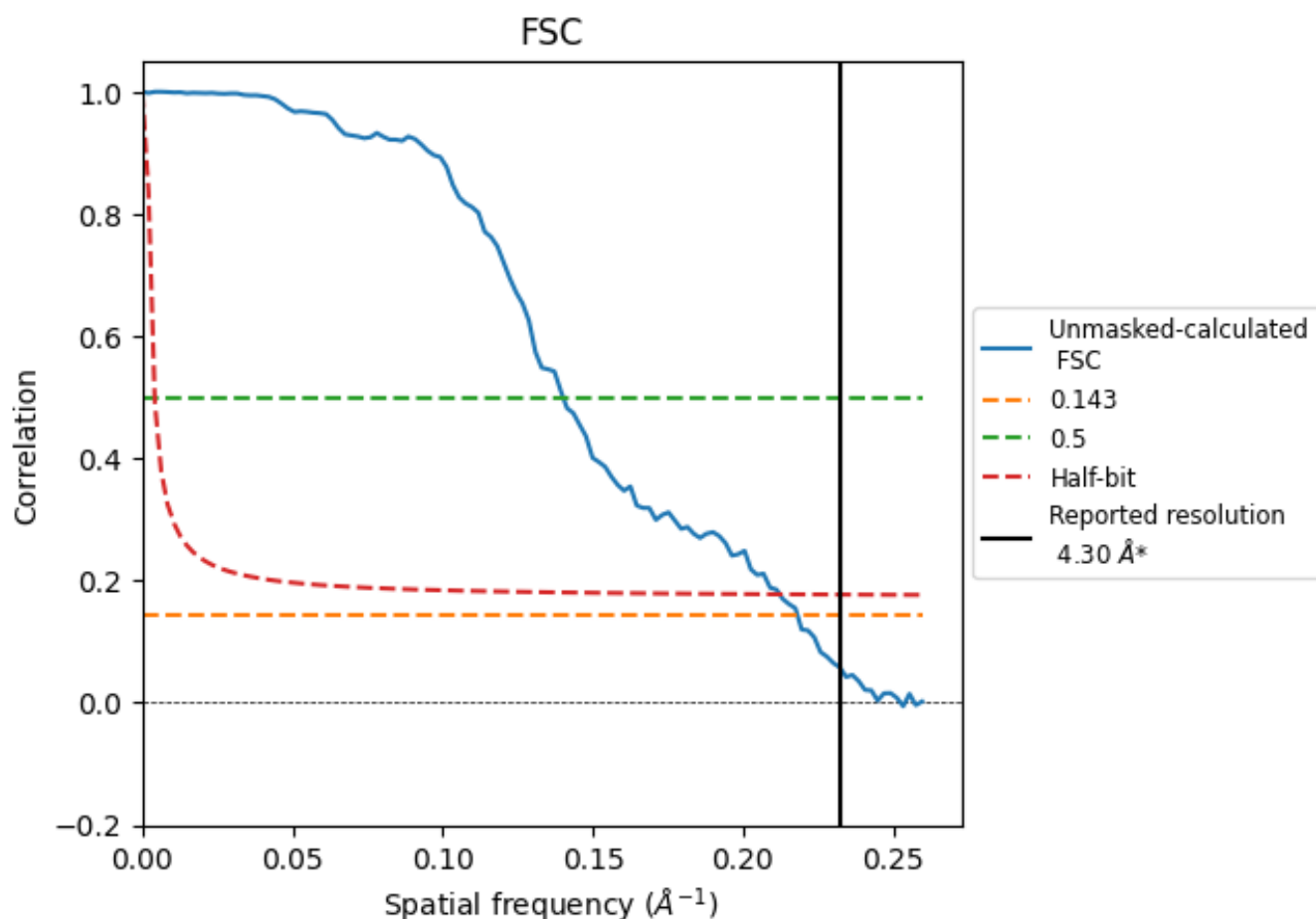


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

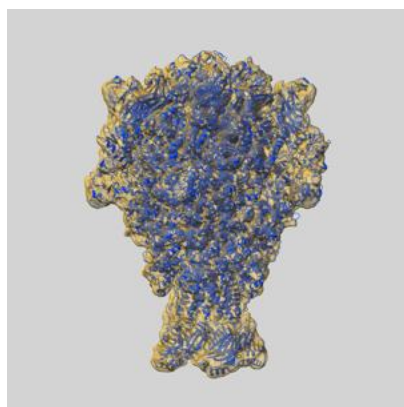
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.59	7.14	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

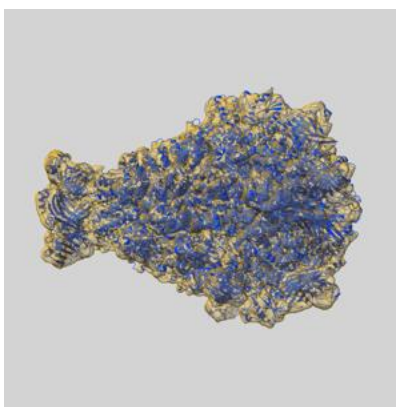
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48371 and PDB model 9MLG. Per-residue inclusion information can be found in section [3](#) on page [20](#).

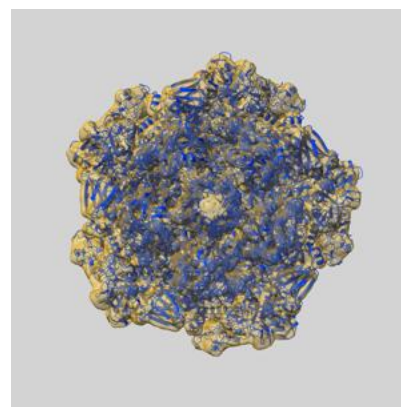
9.1 Map-model overlay [i](#)



X



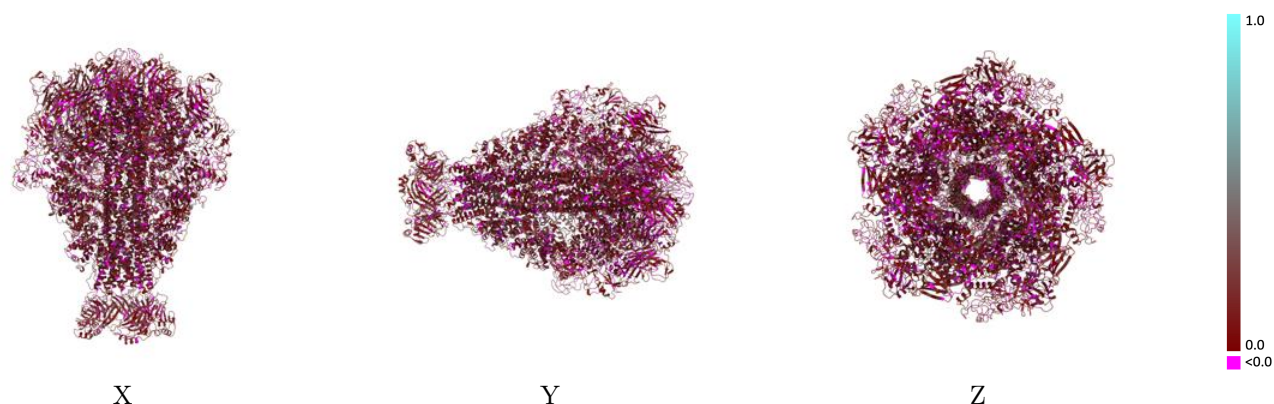
Y



Z

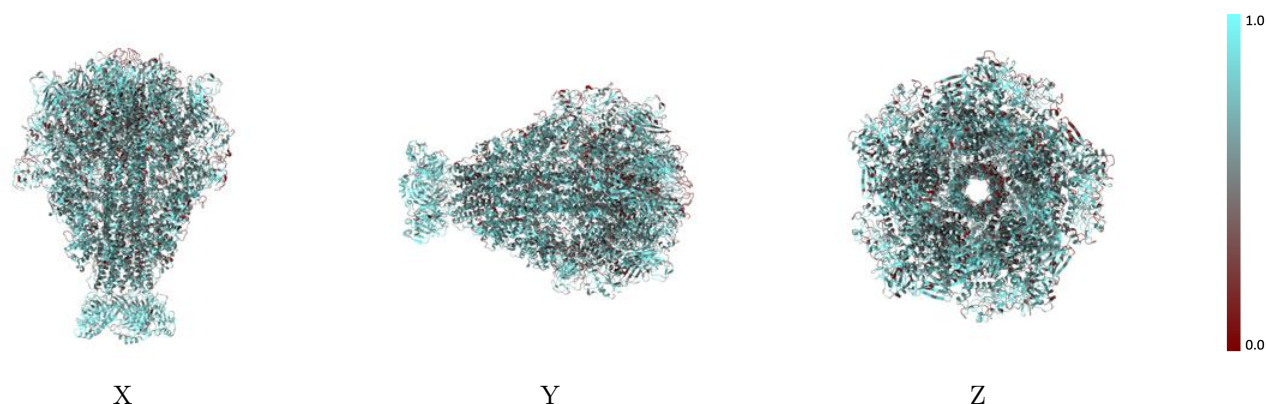
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



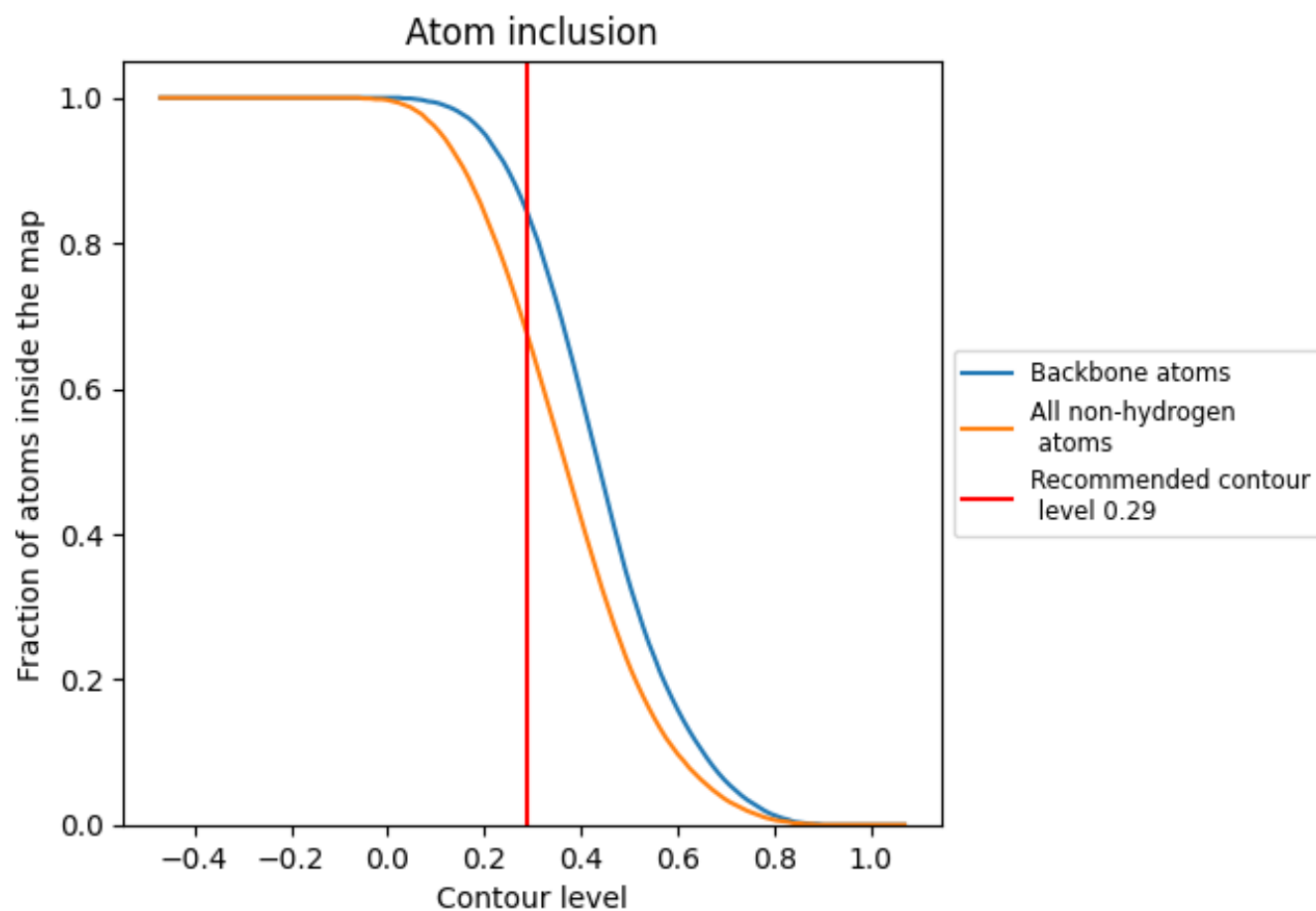
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.1370
A	0.6740	0.1390
B	0.6600	0.1280
C	0.6610	0.1250
D	0.6610	0.1310
E	0.7010	0.1610

