



Full wwPDB EM Validation Report (i)

Jan 7, 2025 – 12:26 PM EST

PDB ID : 9MLG
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 (i) 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 \(i\)](#)) were used in the production of this report:

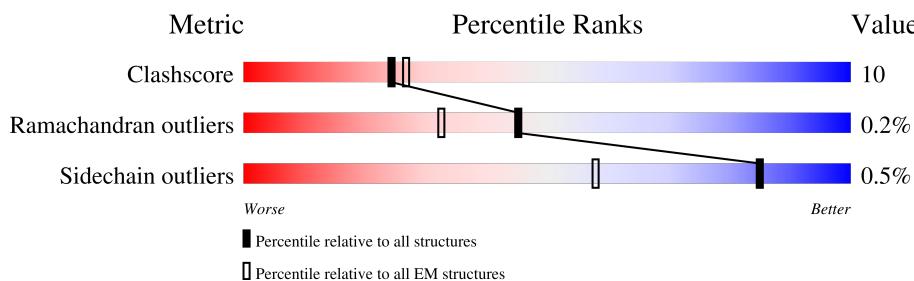
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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.



2 Entry composition (i)

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	C	N	O	S	0	0
			20041	12651	3420	3897	73		
1	B	2540	Total	C	N	O	S	0	0
			20041	12651	3420	3897	73		
1	C	2540	Total	C	N	O	S	0	0
			20041	12651	3420	3897	73		
1	D	2540	Total	C	N	O	S	0	0
			20041	12651	3420	3897	73		
1	E	2540	Total	C	N	O	S	0	0
			20041	12651	3420	3897	73		

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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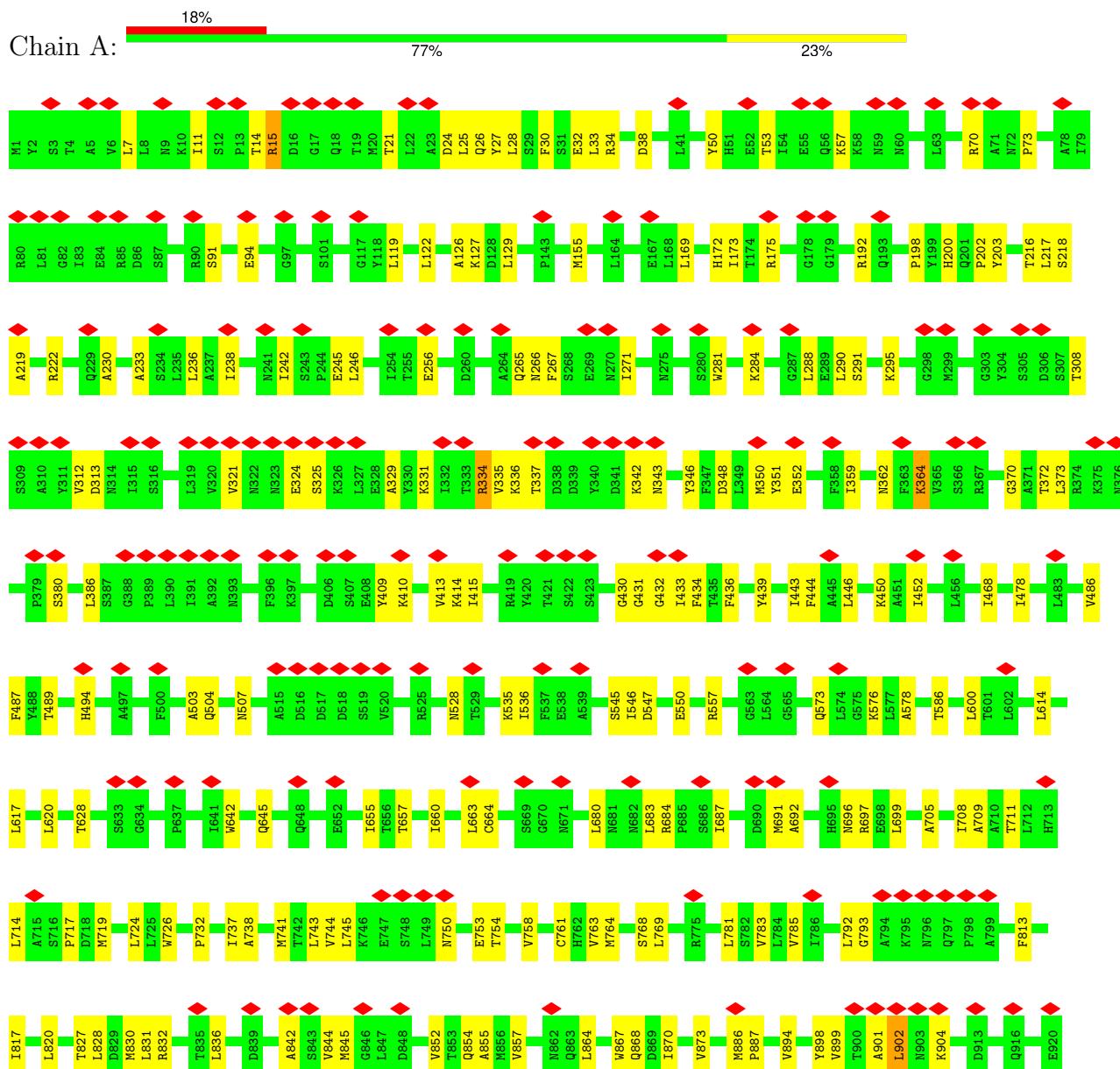
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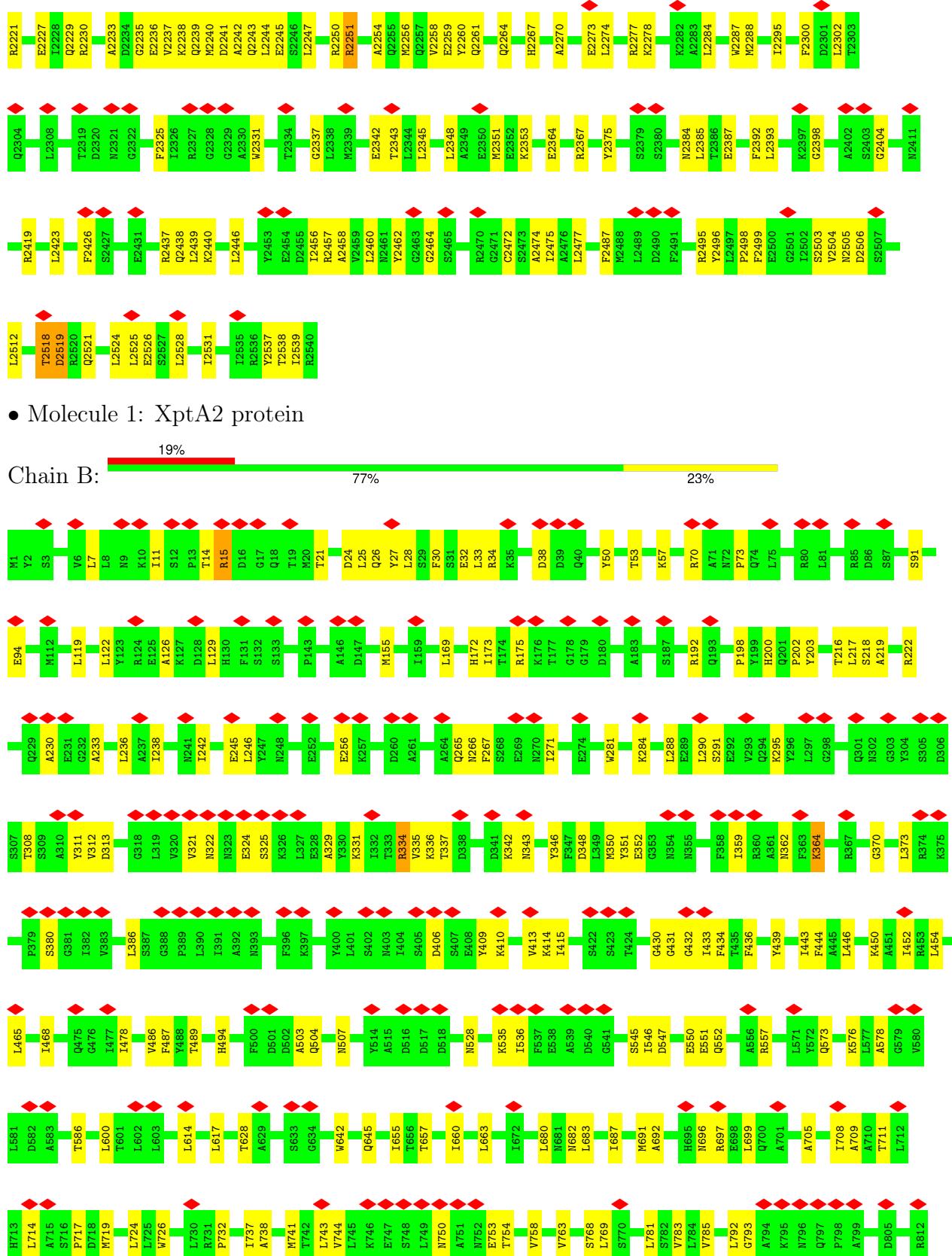
Chain	Residue	Modelled	Actual	Comment	Reference
E	1946	GLY	VAL	conflict	UNP Q93RN7
E	1950	GLN	HIS	conflict	UNP Q93RN7
E	1962	MET	ALA	conflict	UNP Q93RN7
E	1964	GLY	ASP	conflict	UNP Q93RN7
E	1965	ARG	ASN	conflict	UNP Q93RN7
E	1967	GLY	GLU	conflict	UNP Q93RN7
E	1969	SER	ALA	conflict	UNP Q93RN7
E	1970	LYS	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

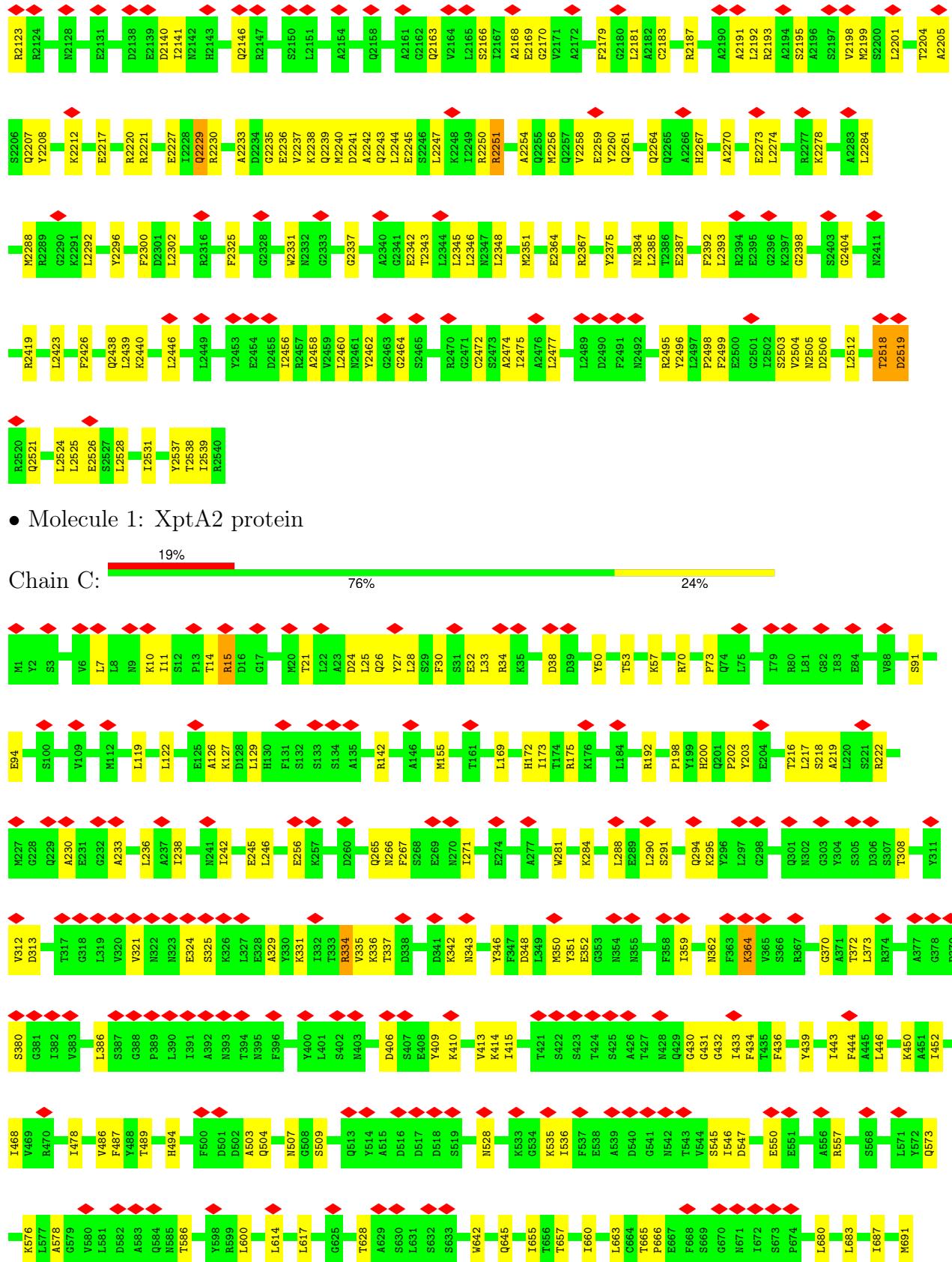
3 Residue-property plots

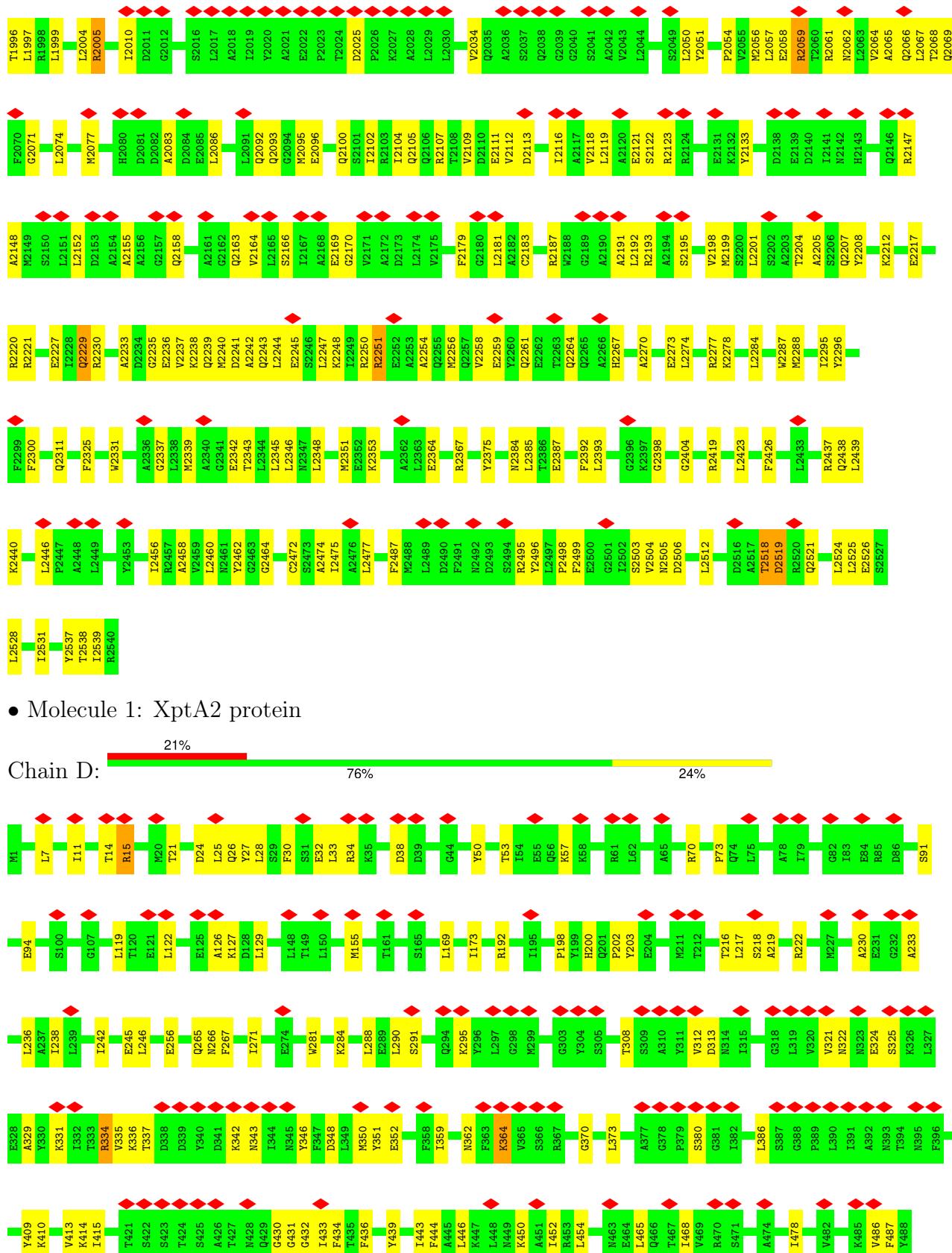
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

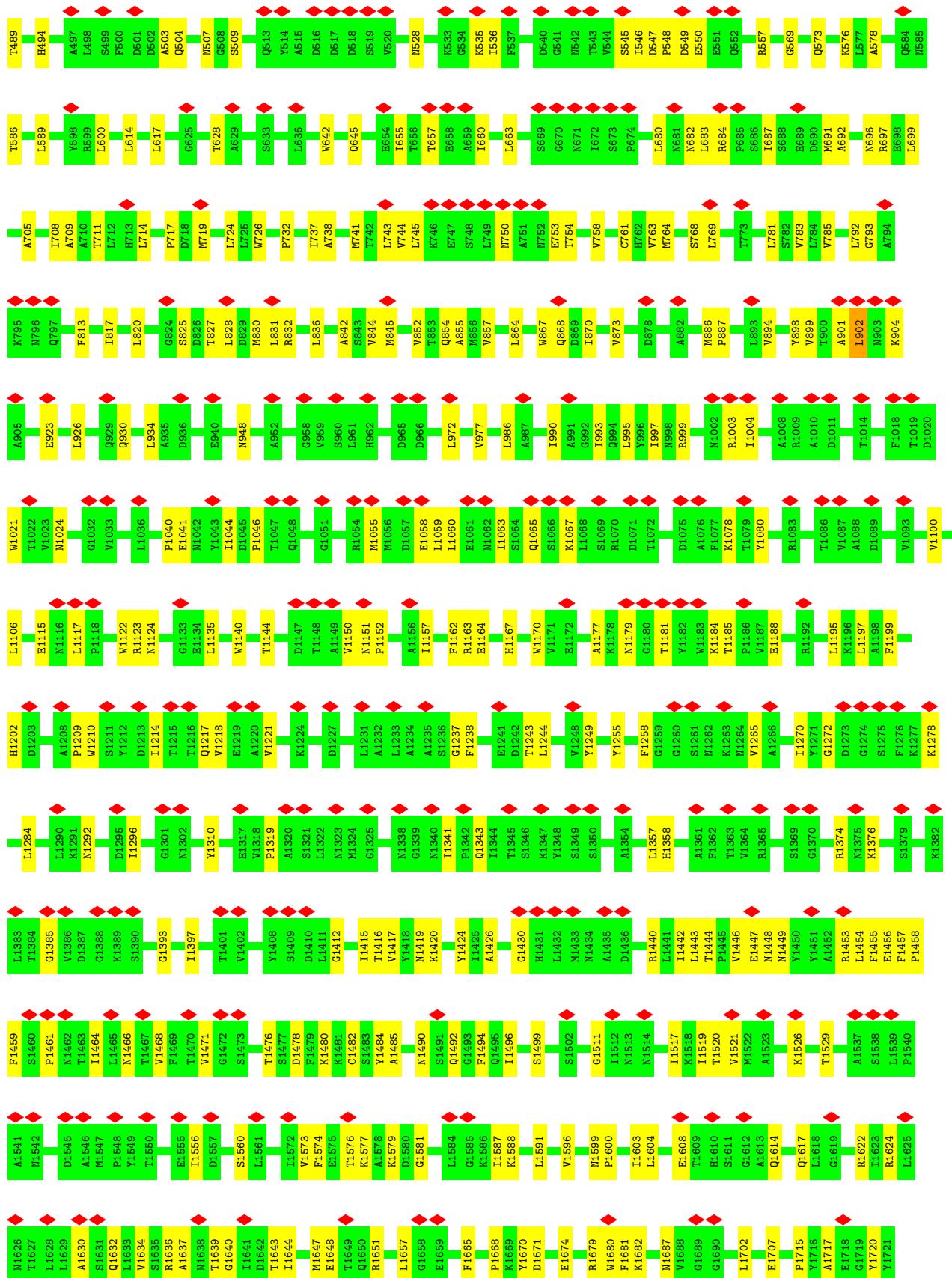
- Molecule 1: XptA2 protein

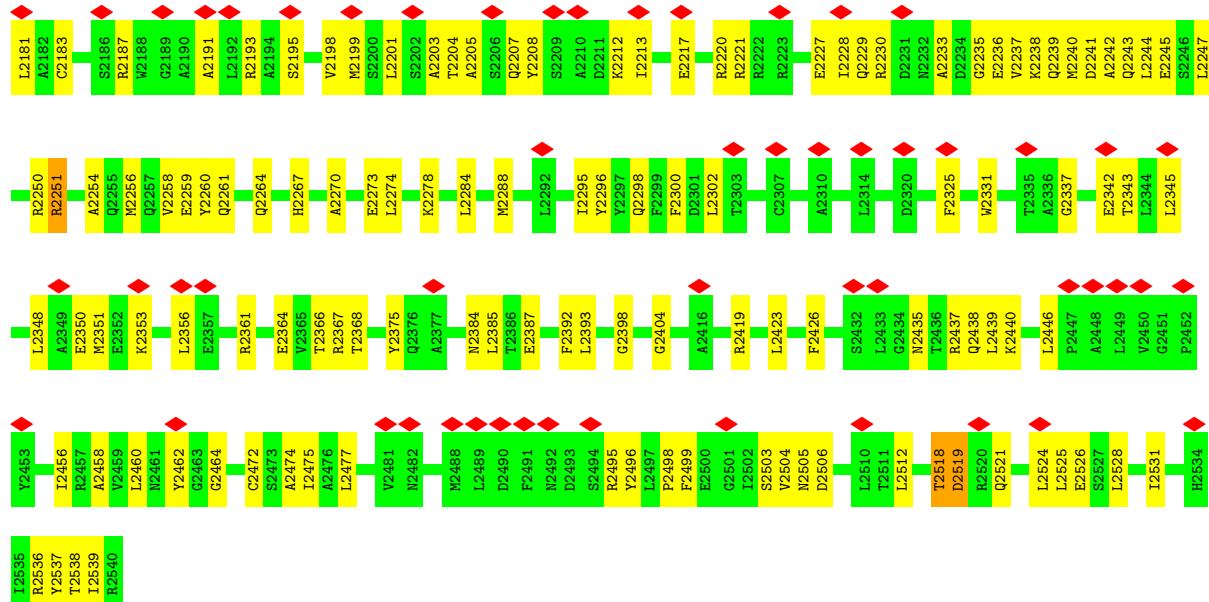
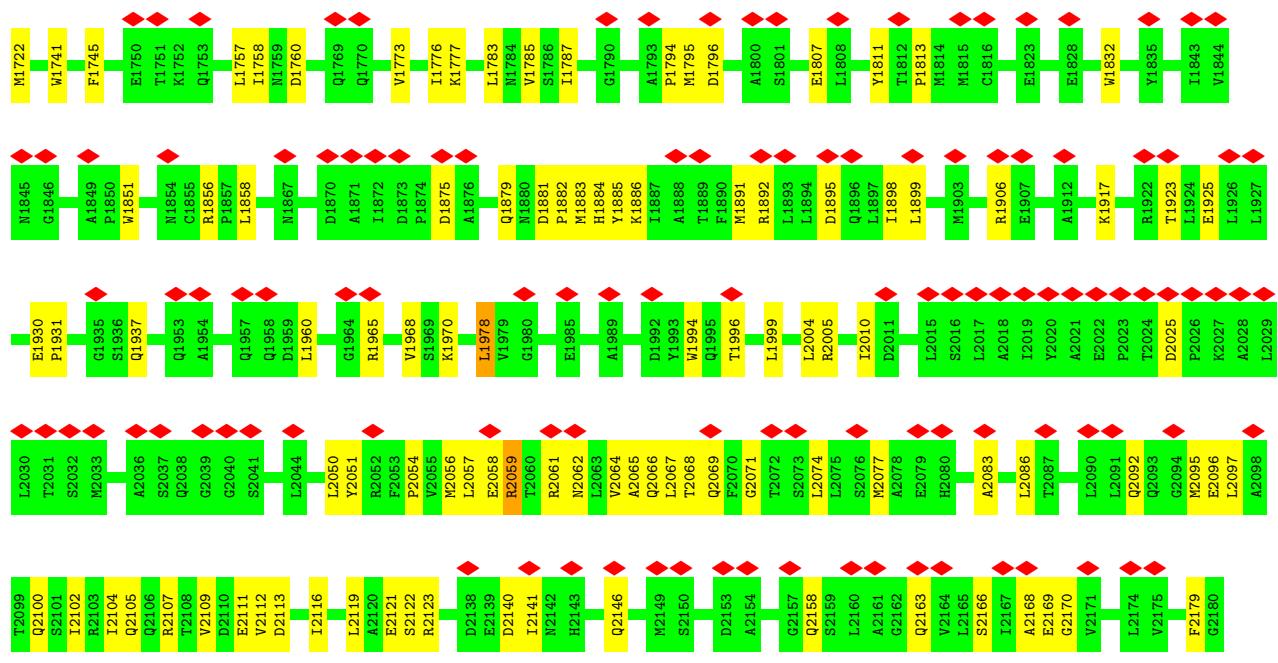




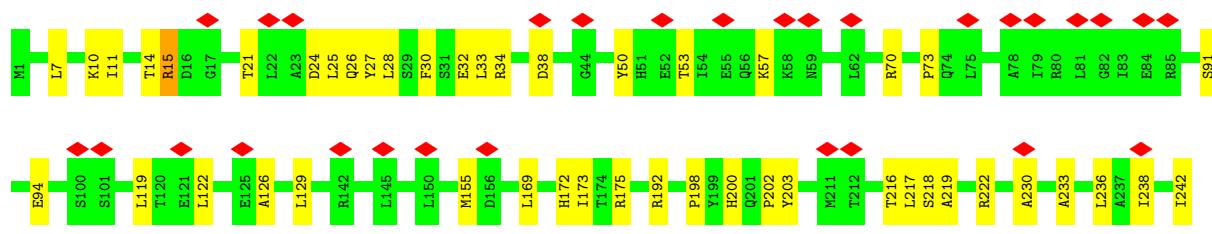


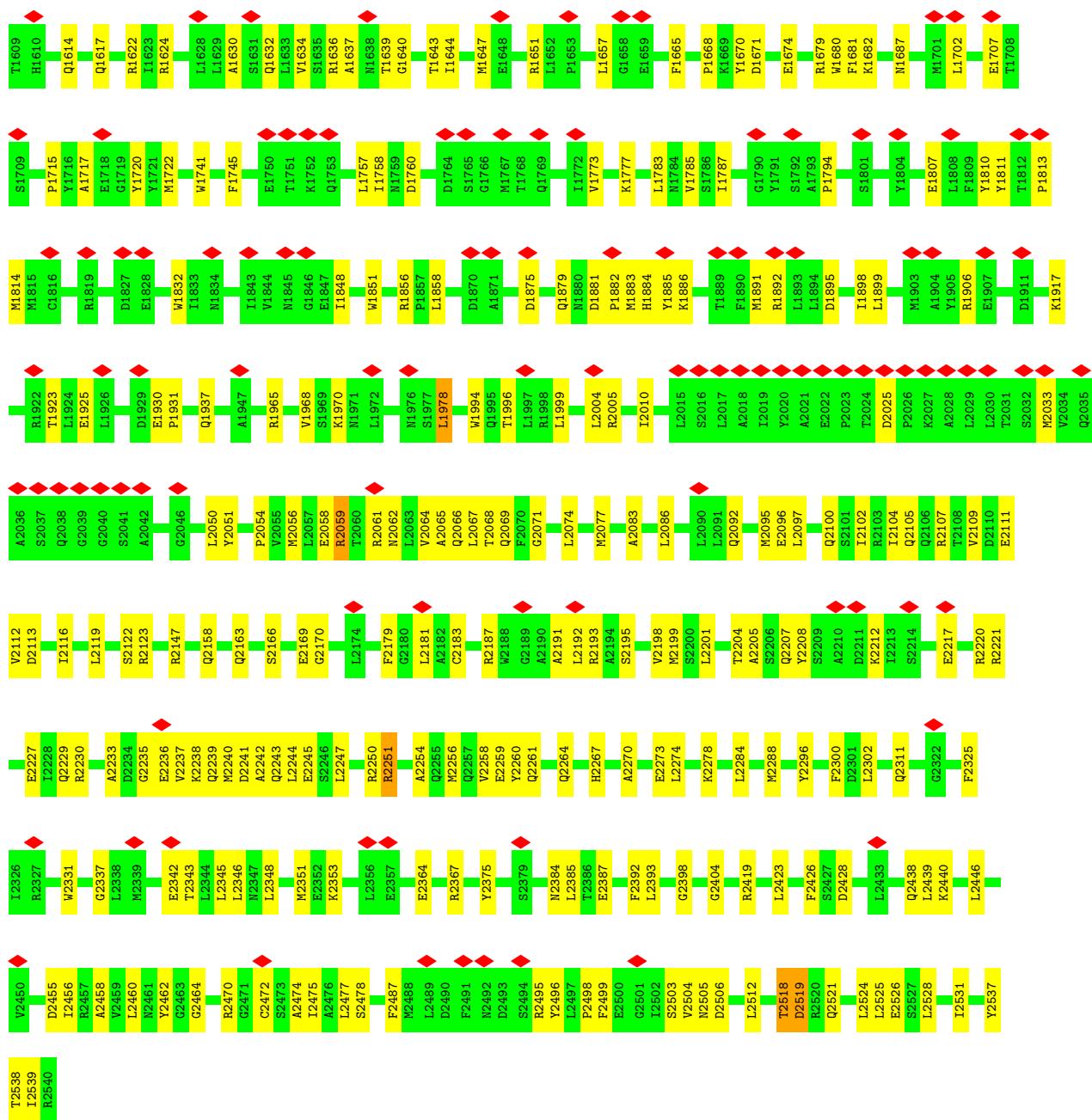






- Molecule 1: XptA2 protein





4 Experimental information (i)

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	0.25	0/20450	0.52	3/27765 (0.0%)
1	B	0.25	0/20450	0.52	3/27765 (0.0%)
1	C	0.25	0/20450	0.52	3/27765 (0.0%)
1	D	0.25	0/20450	0.52	3/27765 (0.0%)
1	E	0.25	0/20450	0.52	3/27765 (0.0%)
All	All	0.25	0/102250	0.52	15/138825 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	2518	THR	C-N-CA	6.85	138.83	121.70
1	B	2518	THR	C-N-CA	6.84	138.80	121.70
1	C	2518	THR	C-N-CA	6.84	138.79	121.70
1	A	2518	THR	C-N-CA	6.83	138.77	121.70
1	E	2518	THR	C-N-CA	6.82	138.75	121.70
1	B	902	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	902	LEU	CA-CB-CG	5.54	128.03	115.30
1	D	902	LEU	CA-CB-CG	5.53	128.02	115.30
1	E	902	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	902	LEU	CA-CB-CG	5.51	127.98	115.30
1	D	1978	LEU	CA-CB-CG	5.13	127.09	115.30
1	C	1978	LEU	CA-CB-CG	5.12	127.07	115.30
1	E	1978	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	1978	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	1978	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	420	0
1	B	20041	0	19627	432	0
1	C	20041	0	19627	464	0
1	D	20041	0	19627	479	0
1	E	20041	0	19627	438	0
All	All	100205	0	98135	2073	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 10.

All (2073) 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: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: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:A:334:ARG:HG3	1:A:415:ILE:HG13	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:LEU:HD23	1:D:744:VAL:HG11	1.62	0.81
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:B:2212:LYS:HZ1	1:E:1065:GLN:HG3	1.48	0.78
1:C:2158:GLN:HG2	1:D:2199:MET:HE1	1.67	0.76
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:26:GLN:HB3	1:C:27:TYR:HA	1.75	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:750:ASN:HB2	1:E:754:THR:HG23	1.79	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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:ALA:HA	1:B:129:LEU:HD23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:2325:PHE:HB2	1:D:2351:MET:HE2	1.82	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:B:2325:PHE:HB2	1:B:2351:MET:HE2	1.83	0.61
1:D:792:LEU:HA	1:D:867:TRP:HB3	1.82	0.61
1:A:2325:PHE:HB2	1:A:2351:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1065:GLN:HG3	1:D:2212:LYS:HZ1	1.65	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
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:B:2033:MET:HE1	1:C:2277:ARG:HH21	1.66	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:A:2212:LYS:HZ1	1:D:1065:GLN:HG3	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB3	1:A:993:ILE:HG21	1.82	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:C:2325:PHE:HB2	1:C:2351:MET:HE2	1.84	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:2158:GLN:O	1:D:2199:MET:HE1	2.03	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:E:2325:PHE:HB2	1:E:2351:MET:HE2	1.85	0.58
1:A:1444:THR:HB	1:A:1453:ARG:HA	1.84	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.86	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:GLN:HE21	1:A:1278:LYS:HE2	1.68	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: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
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:A:2277:ARG:HH21	1:E:2033:MET:HE1	1.70	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2170:GLY:HA3	1:B:2191:ALA:HA	1.87	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: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
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.88	0.55
1:A:348:ASP:HB2	1:A:359:ILE:HG21	1.88	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: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: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: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:C:1065:GLN:HG3	1:E:2212:LYS:HZ1	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:1520:THR:HG22	1:E:1529:THR:HG23	1.88	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: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: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:2059:ARG:HA	1:C:2062:ASN:ND2	2.23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:2158:GLN:HG2	1:B:2199:MET:HE1	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:697:ARG:HG2	1:E:737:ILE:HD12	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2212:LYS:NZ	1:E:1065:GLN:HG3	2.21	0.52
1:B:2375:TYR:HD2	1:B:2385:LEU:HD13	1.74	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:GLN:O	1:A:1636:ARG:HG2	2.10	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:E:2375:TYR:HD2	1:E:2385:LEU:HD13	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
1:D:334:ARG:CB	1:D:434:PHE:HA	2.39	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:A:2518:THR:HB	1:A:2519:ASP:CG	2.31	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:545:SER:HB2	1:B:586:THR:HG22	1.93	0.51
1:B:2518:THR:HB	1:B:2519:ASP:CG	2.31	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:C:2518:THR:HB	1:C:2519:ASP:CG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:D:2518:THR:HB	1:D:2519:ASP:CG	2.31	0.51
1:E:663:LEU:HD11	1:E:769:LEU:HD23	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:844:VAL:HG12	1:D:845:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:844:VAL:HG12	1:E:845:MET:HE2	1.93	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:848:ASP:CG	1:D:569:GLY:HA3	2.31	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:E:1041:GLU:HG3	1:E:1891:MET:HE1	1.94	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
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:886:MET:HE3	1:A:887:PRO:HD2	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:1599:ASN:O	1:C:1603:ILE:HG12	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:844:VAL:HG12	1:C:845:MET:HE2	1.93	0.50
1:E:923:GLU:O	1:E:926:LEU:HD22	2.12	0.50
1:E:2518:THR:HB	1:E:2519:ASP:CG	2.31	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: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:B:886:MET:HE3	1:B:887:PRO:HD2	1.93	0.49
1:E:886:MET:HE3	1:E:887:PRO:HD2	1.94	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
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:B:844:VAL:HG12	1:B:845:MET:HE2	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:D:886:MET:HE3	1:D:887:PRO:HD2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2097:LEU:HD22	1:E:2260:TYR:CE2	2.47	0.49
1:A:1041:GLU:HG3	1:A:1891:MET:HE1	1.95	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: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: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: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: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
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: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:844:VAL:HG12	1:A:845:MET:HE2	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:D:2158:GLN:HG2	1:E:2199:MET:HE1	1.94	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: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:E:726:TRP:NE1	1:E:785:VAL:HG22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:2123:ARG:HB2	1:D:2240:MET:HE1	1.96	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
1:A:413:VAL:HG12	1:A:433:ILE:HD12	1.94	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: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:A:2518:THR:HB	1:A:2519:ASP:OD2	2.13	0.48
1:B:1067:LYS:HZ1	1:D:2140:ASP:HB3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1167:HIS:ND1	1:C:1199:PHE:HB3	2.28	0.47
1:C:2123:ARG:HB2	1:C:2240:MET:HE1	1.96	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: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
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: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:70:ARG:HH12	1:A:1883:MET:CE	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:70:ARG:HH12	1:D:1883:MET:HE2	1.80	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
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:2123:ARG:HB2	1:A:2240:MET:HE1	1.96	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:2119:LEU:HG	1:A:2240:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1123:ARG:HD3	1:C:1140:TRP:HE3	1.80	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:70:ARG:HH12	1:E:1883:MET:HE2	1.80	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: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
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: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:B:2123:ARG:HB2	1:B:2240:MET:HE1	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: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:813:PHE:O	1:D:817:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:2074:LEU:HA	1:C:2077:MET:HG3	1.97	0.46
1:C:2169:GLU:CD	1:D:2193:ARG:HD3	2.36	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: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: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:25:LEU:HA	1:B:27:TYR:HB2	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:2472:CYS:SG	1:D:2498:PRO:HA	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2119:LEU:HG	1:C:2240:MET:HE2	1.98	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1214:ILE:HG22	1:B:1217:GLN:HB2	1.98	0.45
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: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:1065:GLN:HG3	1:C:2212:LYS:HZ1	1.81	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:C:2158:GLN:O	1:D:2199:MET:CE	2.64	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:B:2119:LEU:HG	1:B:2240:MET:HE2	1.98	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: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:2119:LEU:HG	1:D:2240:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2311:GLN:HG3	1:E:2351:MET:HE3	1.99	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:C:2404:GLY:HA3	1:C:2419:ARG:HE	1.80	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: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: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:1810:TYR:CE2	1:E:1814:MET:HE1	2.52	0.44
1:E:1882:PRO:O	1:E:1885:TYR:HB2	2.17	0.44
1:E:2119:LEU:HG	1:E:2240:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:ILE:HG12	1:A:1420:LYS:HZ2	1.83	0.44
1:B:351:TYR:HB2	1:B:409:TYR:HE1	1.82	0.44
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.85	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:886:MET:HE3	1:C:887:PRO:HD2	1.99	0.44
1:C:1078:LYS:HE2	1:D:1202:HIS:HB3	1.99	0.44
1:C:2158:GLN:HG2	1:D:2199:MET:CE	2.44	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: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:B:655:ILE:HG21	1:B:660:ILE:HD13	2.00	0.44
1:B:1041:GLU:HG3	1:B:1891:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:2123:ARG:HB2	1:E:2240:MET:HE1	1.98	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:864:LEU:HD12	1:D:864:LEU:O	2.18	0.44
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:B:70:ARG:HH12	1:B:1883:MET:HE2	1.82	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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1040:PRO:O	1:C:1044:ILE:HG12	2.18	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1397:ILE:HG12	1:B:1420:LYS:HZ2	1.84	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: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
1:A:2141:ILE:H	1:D:1067:LYS:HZ2	1.67	0.43
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:1397:ILE:HG12	1:D:1420:LYS:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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: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: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:1397:ILE:HG12	1:C:1420:LYS:HZ2	1.83	0.42
1:C:2061:ARG:HG3	1:C:2348:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:2199:MET:HE1	1:E:2158:GLN:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1520:THR:OG1	1:B:1573:VAL:HB	2.19	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
1:E:1397:ILE:HG12	1:E:1420:LYS:HZ2	1.83	0.42
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:372:THR:HA	1:C:414:LYS:HZ1	1.84	0.42
1:C:2311:GLN:HG3	1:C:2351:MET:HE3	2.01	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:172:HIS:CE1	1:A:175:ARG:HH21	2.38	0.42
1:A:372:THR:HA	1:A:414:LYS:HZ1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2066:GLN:HA	1:C:2069:GLN:CD	2.41	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
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:B:2066:GLN:HA	1:B:2069:GLN:CD	2.41	0.41
1:C:573:GLN:HA	1:C:576:LYS:HE2	2.02	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:2066:GLN:HA	1:A:2069:GLN:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:14:THR:C	1:D:15:ARG:HD3	2.41	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: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: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: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:14:THR:C	1:C:15:ARG:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:70:ARG:HH12	1:A:1883:MET:HE2	1.85	0.41
1:B:14:THR:C	1:B:15:ARG:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2066:GLN:HA	1:D:2069:GLN:CD	2.41	0.41
1:D:2537:TYR:HE2	1:D:2539:ILE:HD11	1.86	0.41
1:E:14:THR:C	1:E:15:ARG:HD3	2.41	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
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: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:2212:LYS:HZ1	1:E:1065:GLN:CG	2.27	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:1795:MET:HE3	1:C:1796:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1059:LEU:HD22	1:D:1080:TYR:CD1	2.55	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: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
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:1041:GLU:HG3	1:C:1891:MET:HE1	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: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:1041:GLU:HG3	1:D:1891:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:D:1795:MET:HE3	1:D:1796:ASP:O	2.21	0.41
1:E:321:VAL:HG11	1:E:324:GLU:HB3	2.03	0.41
1:A:14:THR:C	1:A:15:ARG:HD3	2.41	0.40
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:1795:MET:HE3	1:B:1796:ASP: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2066:GLN:HA	1:E:2069:GLN:CD	2.41	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
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:2158:GLN:HE21	1:E:2199:MET:CE	2.33	0.40
1:D:2274:LEU:O	1:D:2278:LYS:HG2	2.21	0.40
1:D:2342:GLU:HG2	1:D:2343:THR:N	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:761:CYS:HA	1:A:764:MET:HG2	2.02	0.40
1:A:1681:PHE:HD1	1:A:1702:LEU:HG	1.86	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:B:2033:MET:HE1	1:C:2277:ARG:NH2	2.34	0.40
1:C:439:TYR:CD1	1:C:443:ILE:HD12	2.55	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:B:329:ALA:HB3	1:B:444:PHE:CE2	2.55	0.40
1:C:70:ARG:HH12	1:C:1883:MET:HE2	1.86	0.40
1:C:1604:LEU:HA	1:C:1617:GLN:O	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2475:ILE:HG23	1:E:2499:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	44 78
1	B	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	44 78
1	C	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	44 78
1	D	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	44 78
1	E	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	44 78
All	All	12690/12700 (100%)	11872 (94%)	798 (6%)	20 (0%)	45 78

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

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Mol	Chain	Res	Type
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 [\(i\)](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2175/2177 (100%)	2164 (100%)	11 (0%)	86 90
1	B	2175/2177 (100%)	2164 (100%)	11 (0%)	86 90
1	C	2175/2177 (100%)	2164 (100%)	11 (0%)	86 90
1	D	2175/2177 (100%)	2164 (100%)	11 (0%)	86 90
1	E	2175/2177 (100%)	2164 (100%)	11 (0%)	86 90
All	All	10875/10885 (100%)	10820 (100%)	55 (0%)	85 90

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	334	ARG
1	A	364	LYS
1	A	948	ASN
1	A	1374	ARG
1	A	1965	ARG
1	A	2005	ARG
1	A	2059	ARG
1	A	2220	ARG
1	A	2229	GLN
1	A	2251	ARG
1	B	15	ARG

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Mol	Chain	Res	Type
1	B	334	ARG
1	B	364	LYS
1	B	948	ASN
1	B	1374	ARG
1	B	1965	ARG
1	B	2005	ARG
1	B	2059	ARG
1	B	2220	ARG
1	B	2229	GLN
1	B	2251	ARG
1	C	15	ARG
1	C	334	ARG
1	C	364	LYS
1	C	948	ASN
1	C	1374	ARG
1	C	1965	ARG
1	C	2005	ARG
1	C	2059	ARG
1	C	2220	ARG
1	C	2229	GLN
1	C	2251	ARG
1	D	15	ARG
1	D	334	ARG
1	D	364	LYS
1	D	948	ASN
1	D	1374	ARG
1	D	1965	ARG
1	D	2005	ARG
1	D	2059	ARG
1	D	2220	ARG
1	D	2229	GLN
1	D	2251	ARG
1	E	15	ARG
1	E	334	ARG
1	E	364	LYS
1	E	948	ASN
1	E	1374	ARG
1	E	1965	ARG
1	E	2005	ARG
1	E	2059	ARG
1	E	2220	ARG
1	E	2229	GLN

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Mol	Chain	Res	Type
1	E	2251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	345	ASN
1	A	362	ASN
1	A	750	ASN
1	A	1937	GLN
1	A	2261	GLN
1	A	2267	HIS
1	A	2505	ASN
1	B	266	ASN
1	B	345	ASN
1	B	362	ASN
1	B	682	ASN
1	B	750	ASN
1	B	1151	ASN
1	B	1937	GLN
1	B	2261	GLN
1	B	2267	HIS
1	B	2505	ASN
1	C	294	GLN
1	C	362	ASN
1	C	750	ASN
1	C	818	ASN
1	C	2261	GLN
1	C	2267	HIS
1	C	2505	ASN
1	D	266	ASN
1	D	345	ASN
1	D	362	ASN
1	D	682	ASN
1	D	750	ASN
1	D	1151	ASN
1	D	1937	GLN
1	D	2158	GLN
1	D	2239	GLN
1	D	2261	GLN
1	D	2267	HIS
1	D	2298	GLN

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Mol	Chain	Res	Type
1	D	2435	ASN
1	D	2505	ASN
1	E	345	ASN
1	E	362	ASN
1	E	750	ASN
1	E	1151	ASN
1	E	1937	GLN
1	E	2261	GLN
1	E	2267	HIS
1	E	2347	ASN
1	E	2505	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

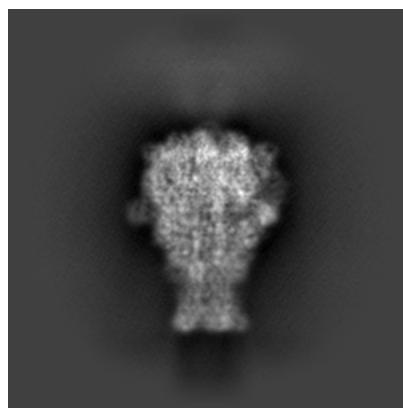
6 Map visualisation (i)

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.

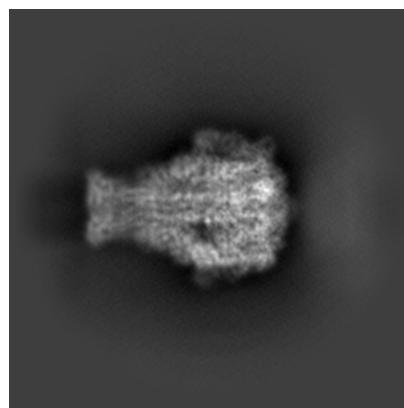
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

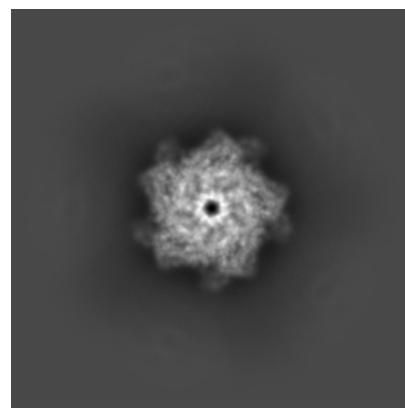
6.1.1 Primary map



X

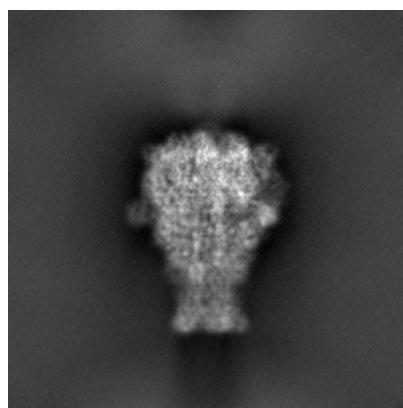


Y

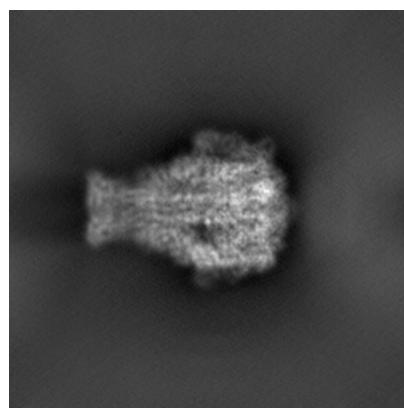


Z

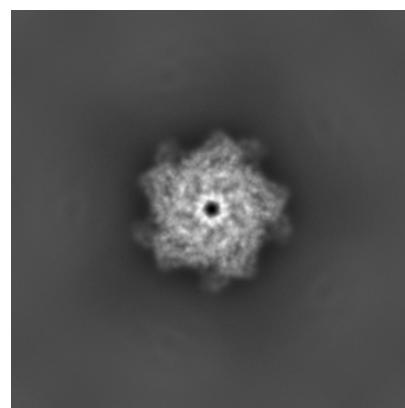
6.1.2 Raw map



X



Y

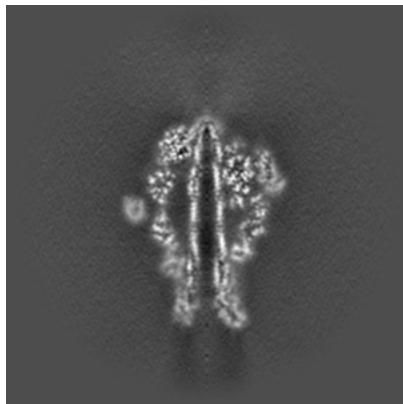


Z

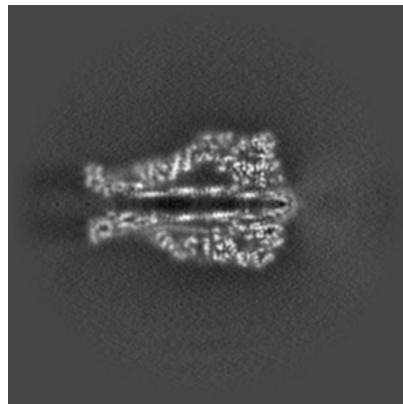
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

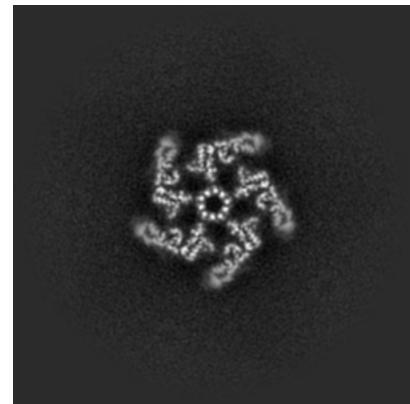
6.2.1 Primary map



X Index: 123

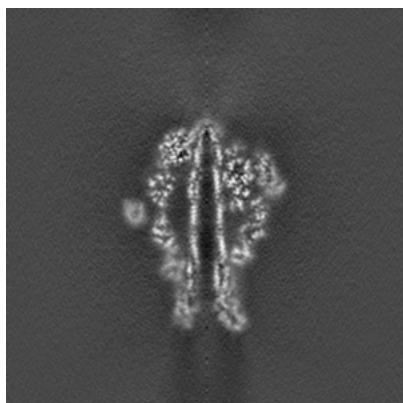


Y Index: 123

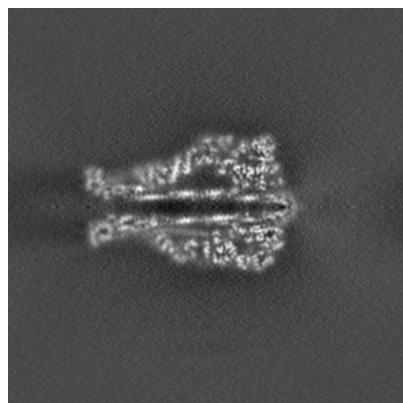


Z Index: 123

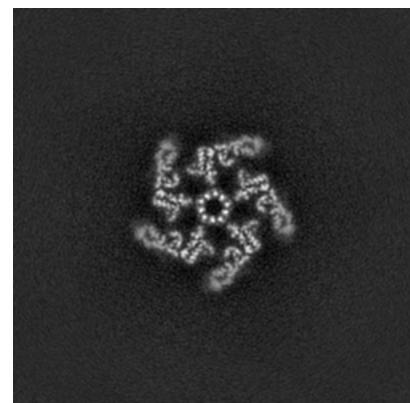
6.2.2 Raw map



X Index: 123



Y Index: 123

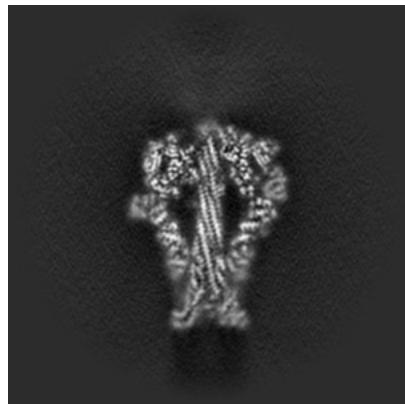


Z Index: 123

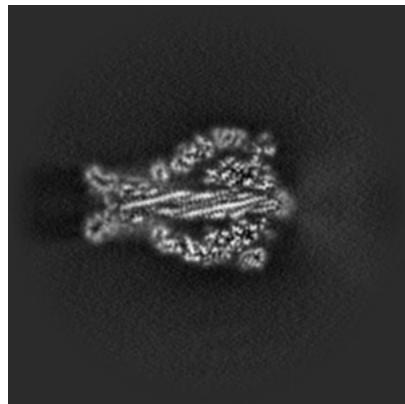
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

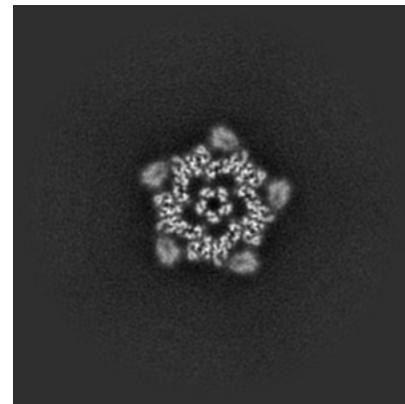
6.3.1 Primary map



X Index: 130

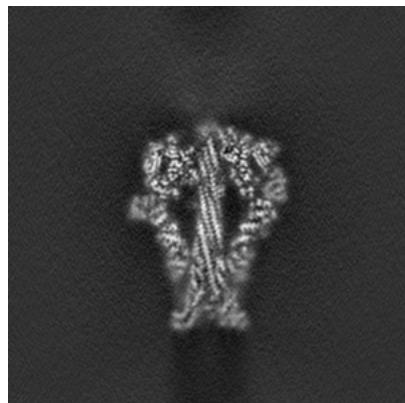


Y Index: 129

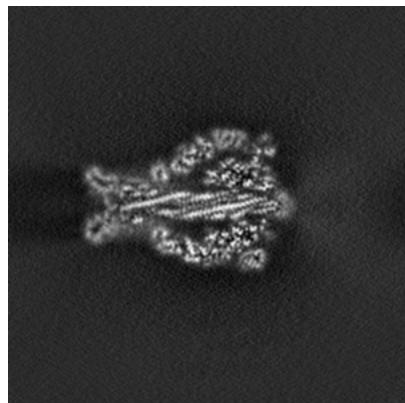


Z Index: 132

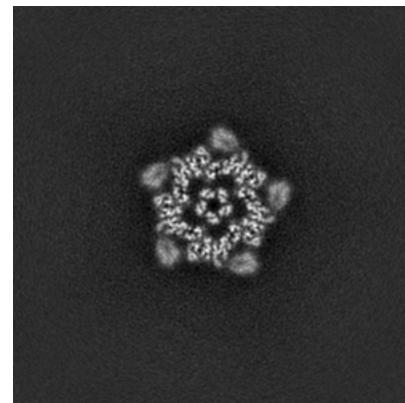
6.3.2 Raw map



X Index: 130



Y Index: 129

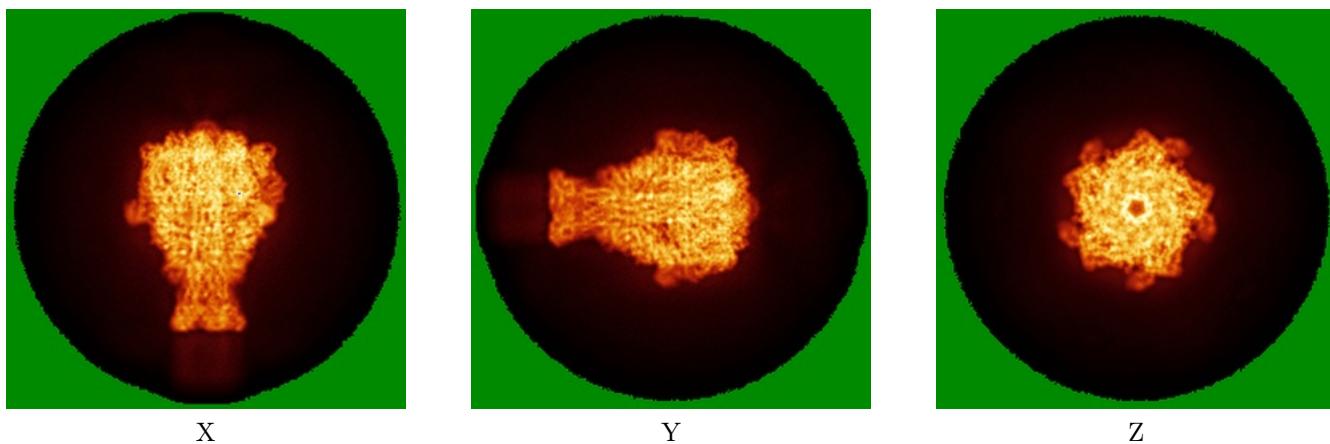


Z Index: 132

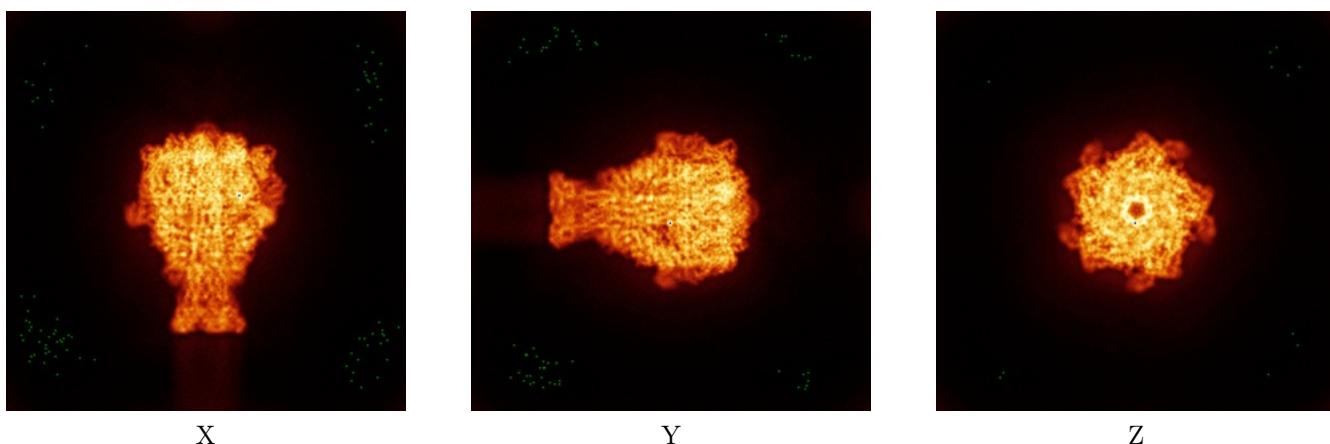
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



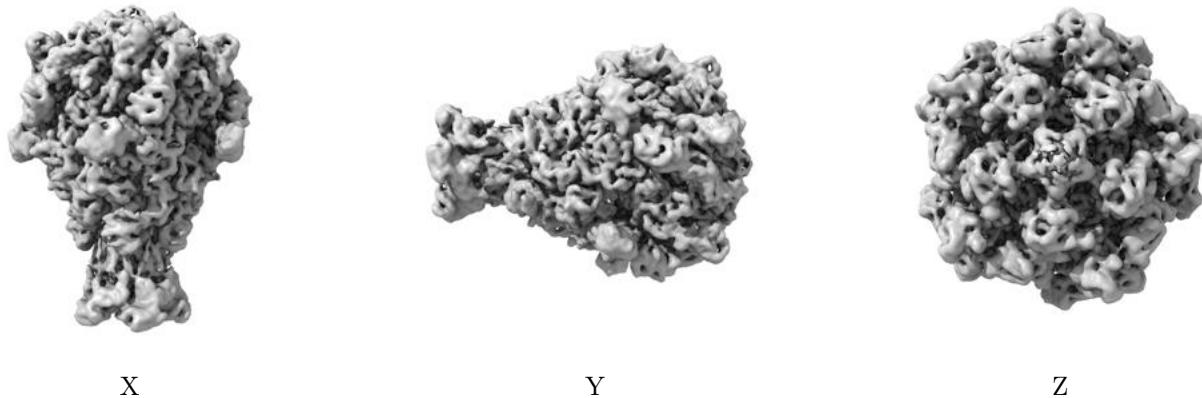
6.4.2 Raw map



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 [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

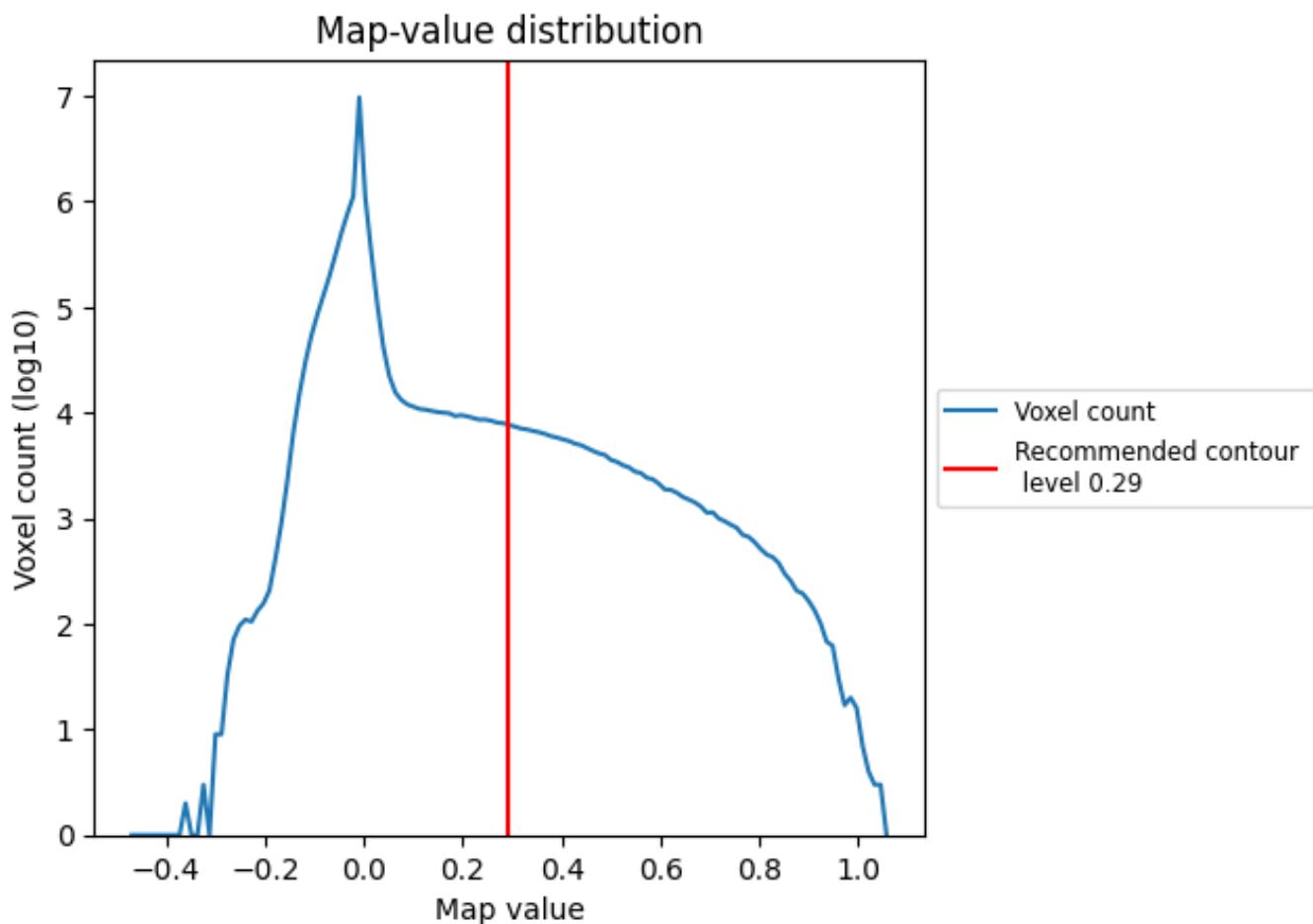
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

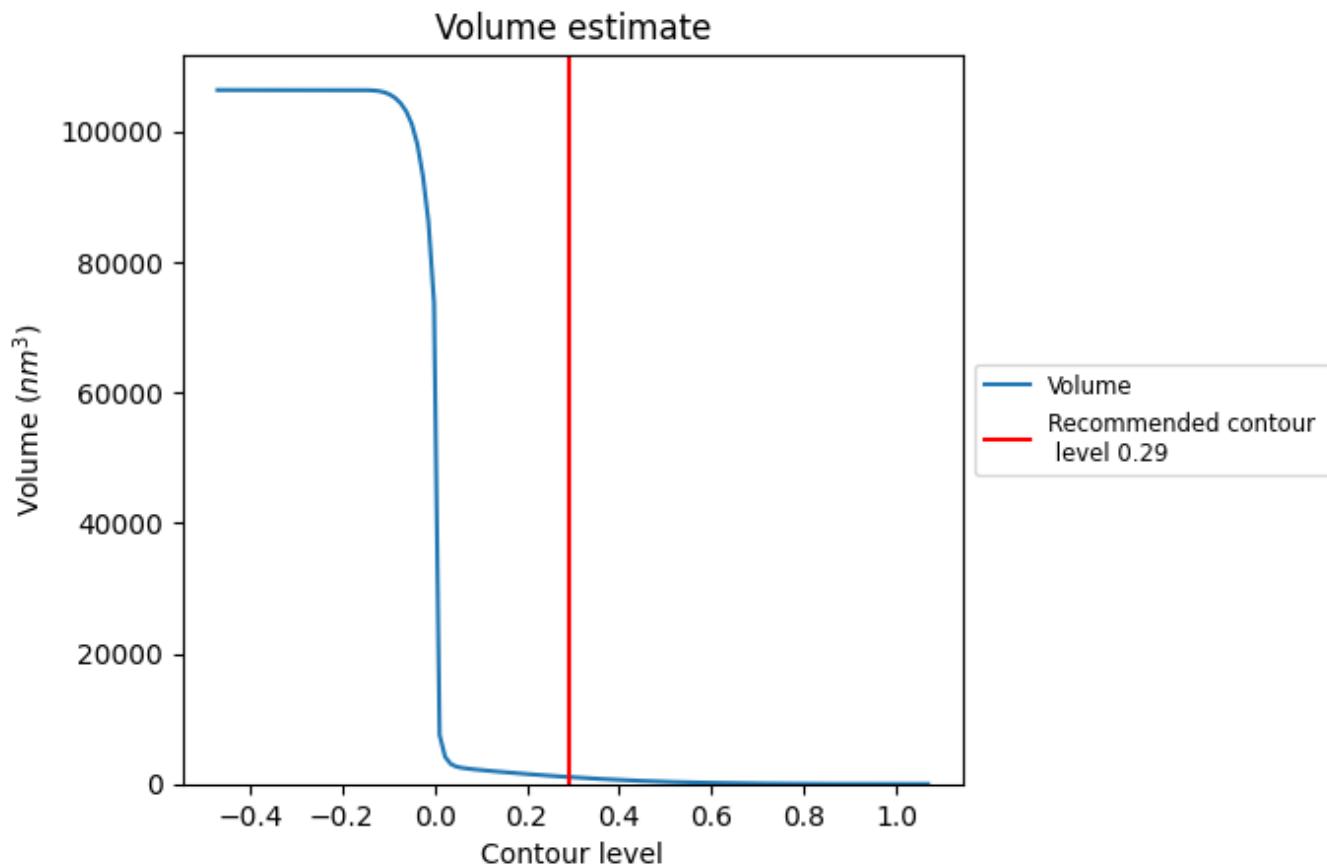
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

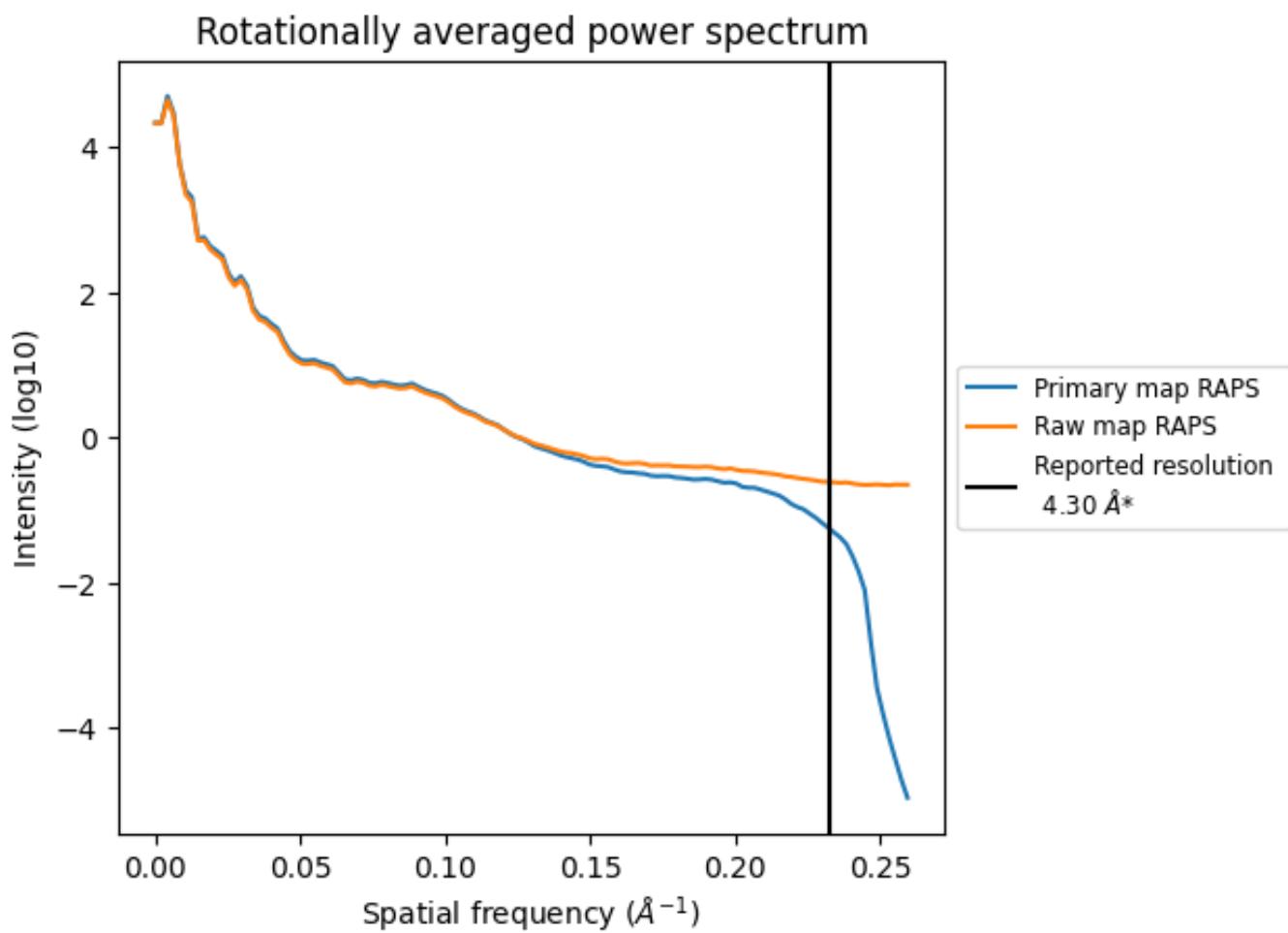
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1065 nm^3 ; 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 [\(i\)](#)

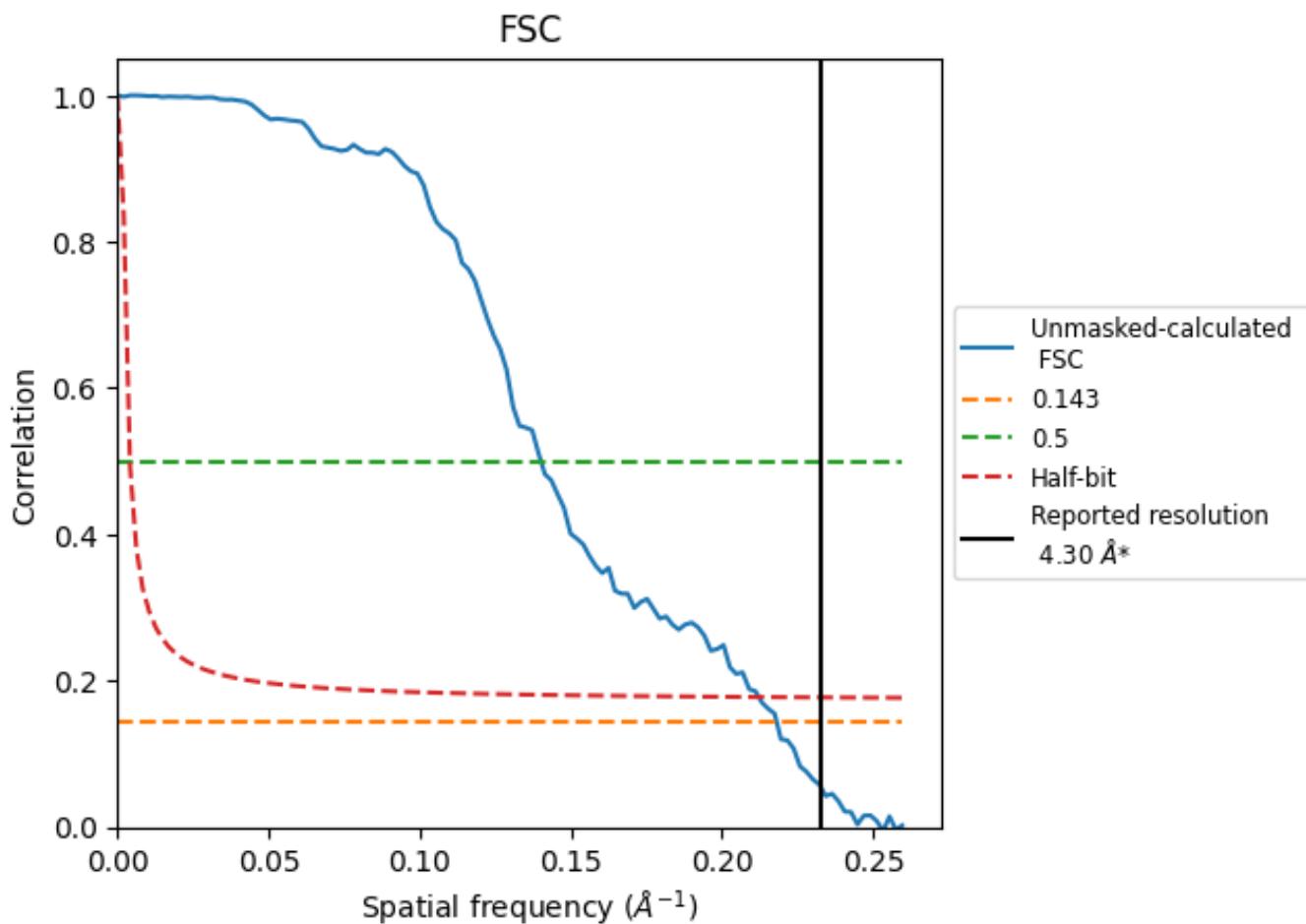


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

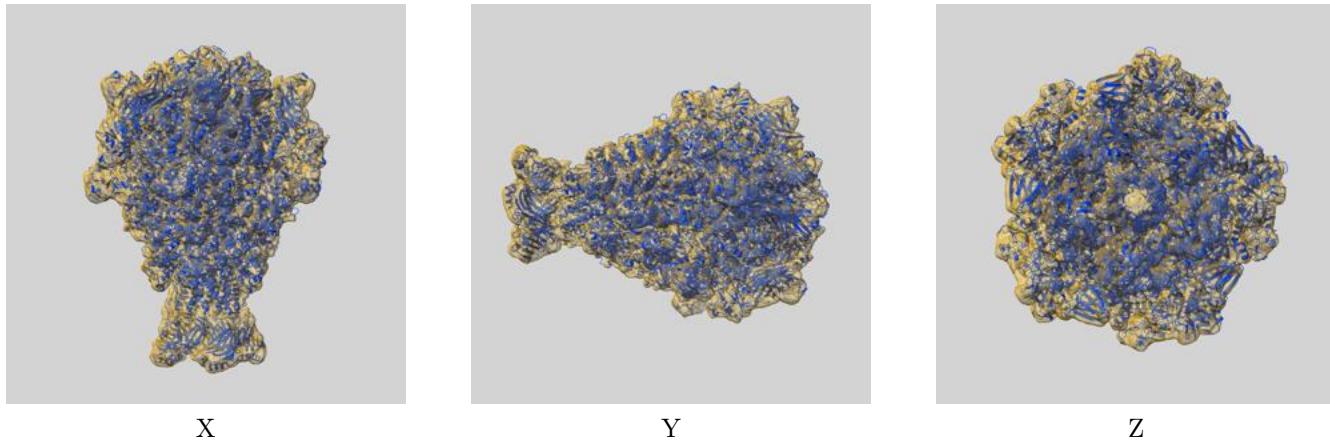
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.59	7.14	4.71

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

9 Map-model fit [\(i\)](#)

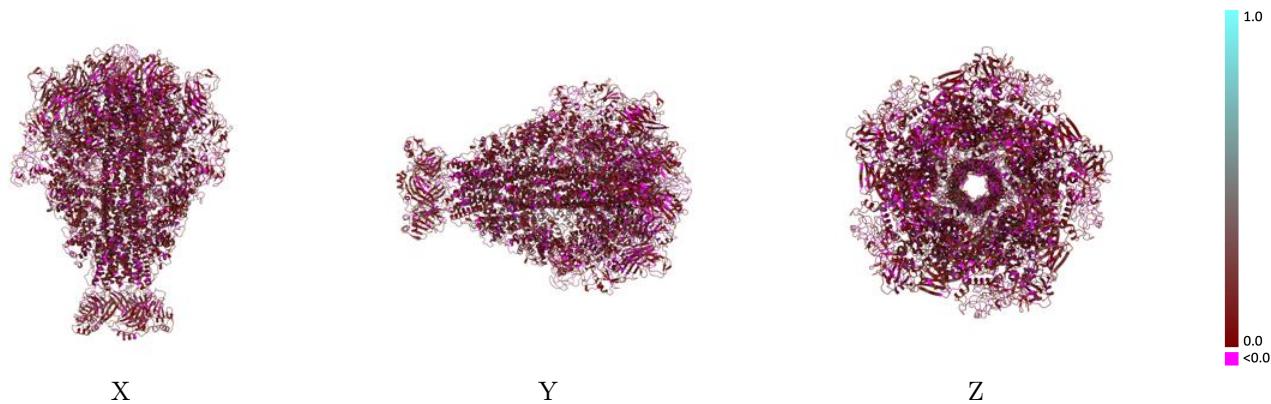
This section contains information regarding the fit between EMDB map EMD-48371 and PDB model 9MLG. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [\(i\)](#)



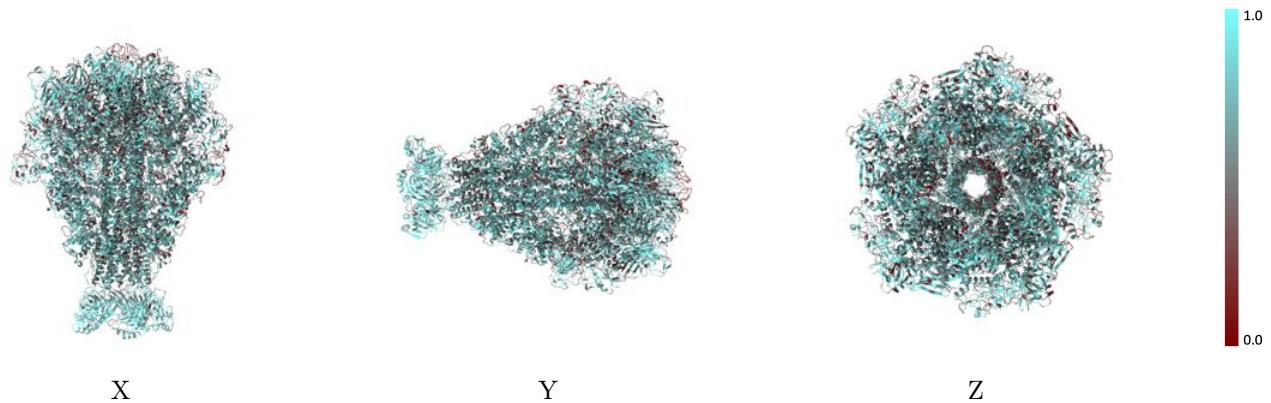
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



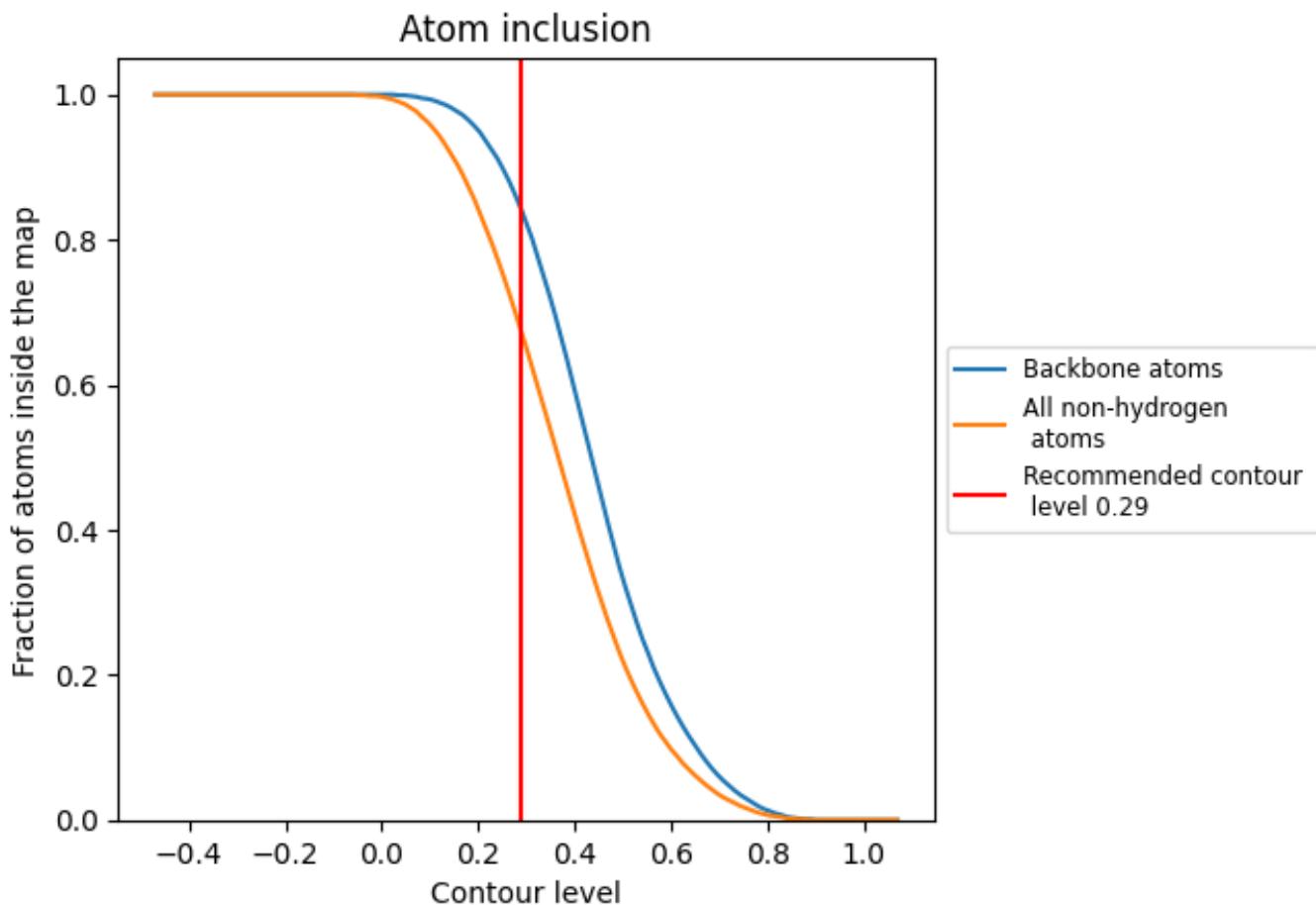
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

