Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:14 pm GMT

PDB ID	:	6G2H
EMDB ID	:	EMD-4343
Title	:	Filament of acetyl-CoA carboxylase and BRCT domains of BRCA1 (ACC-BRCT) core at 4.6 A resolution
Authors	:	Hunkeler, M.; Hagmann, A.; Stuttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on	:	2018-03-23
Resolution	:	4.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

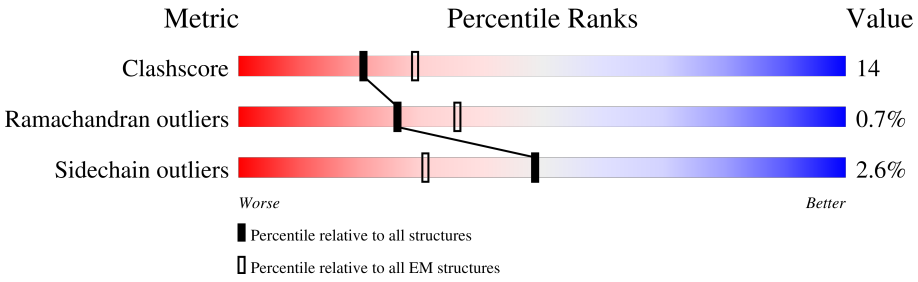
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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.

Mol	Chain	Length	Quality of chain
1	A	2407	10% 20% 11% • 68%
1	B	2407	10% 21% 10% • 68%
1	C	2407	• 28% 10% • 61%
1	D	2407	• 42% 20% • 37%
1	E	2407	• 42% 20% • 37%
1	F	2407	• 28% 11% • 61%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 103896 atoms, of which 51852 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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	1518	Total	C	H	N	O	S	0	0
			24416	7790	12181	2126	2249	70		
1	E	1518	Total	C	H	N	O	S	0	0
			24416	7790	12181	2126	2249	70		
1	C	948	Total	C	H	N	O	S	0	0
			15171	4850	7561	1318	1403	39		
1	F	948	Total	C	H	N	O	S	0	0
			15171	4850	7561	1318	1403	39		
1	B	761	Total	C	H	N	O	S	0	0
			12361	3935	6184	1076	1125	41		
1	A	761	Total	C	H	N	O	S	0	0
			12361	3935	6184	1076	1125	41		

There are 366 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-60	MET	-	initiating methionine	UNP Q13085
D	-59	ALA	-	expression tag	UNP Q13085
D	-58	HIS	-	expression tag	UNP Q13085
D	-57	HIS	-	expression tag	UNP Q13085
D	-56	HIS	-	expression tag	UNP Q13085
D	-55	HIS	-	expression tag	UNP Q13085
D	-54	HIS	-	expression tag	UNP Q13085
D	-53	HIS	-	expression tag	UNP Q13085
D	-52	HIS	-	expression tag	UNP Q13085
D	-51	HIS	-	expression tag	UNP Q13085
D	-50	HIS	-	expression tag	UNP Q13085
D	-49	HIS	-	expression tag	UNP Q13085
D	-48	GLY	-	expression tag	UNP Q13085
D	-47	SER	-	expression tag	UNP Q13085
D	-46	THR	-	expression tag	UNP Q13085
D	-45	SER	-	expression tag	UNP Q13085
D	-44	GLY	-	expression tag	UNP Q13085
D	-43	SER	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-42	GLY	-	expression tag	UNP Q13085
D	-41	GLU	-	expression tag	UNP Q13085
D	-40	GLN	-	expression tag	UNP Q13085
D	-39	LYS	-	expression tag	UNP Q13085
D	-38	LEU	-	expression tag	UNP Q13085
D	-37	ILE	-	expression tag	UNP Q13085
D	-36	SER	-	expression tag	UNP Q13085
D	-35	GLU	-	expression tag	UNP Q13085
D	-34	GLU	-	expression tag	UNP Q13085
D	-33	ASP	-	expression tag	UNP Q13085
D	-32	LEU	-	expression tag	UNP Q13085
D	-31	GLY	-	expression tag	UNP Q13085
D	-30	SER	-	expression tag	UNP Q13085
D	-29	THR	-	expression tag	UNP Q13085
D	-28	SER	-	expression tag	UNP Q13085
D	-27	GLY	-	expression tag	UNP Q13085
D	-26	SER	-	expression tag	UNP Q13085
D	-25	GLY	-	expression tag	UNP Q13085
D	-24	ASP	-	expression tag	UNP Q13085
D	-23	TYR	-	expression tag	UNP Q13085
D	-22	LYS	-	expression tag	UNP Q13085
D	-21	ASP	-	expression tag	UNP Q13085
D	-20	ASP	-	expression tag	UNP Q13085
D	-19	ASP	-	expression tag	UNP Q13085
D	-18	ASP	-	expression tag	UNP Q13085
D	-17	LYS	-	expression tag	UNP Q13085
D	-16	LEU	-	expression tag	UNP Q13085
D	-15	THR	-	expression tag	UNP Q13085
D	-14	SER	-	expression tag	UNP Q13085
D	-13	LEU	-	expression tag	UNP Q13085
D	-12	TYR	-	expression tag	UNP Q13085
D	-11	LYS	-	expression tag	UNP Q13085
D	-10	LYS	-	expression tag	UNP Q13085
D	-9	ALA	-	expression tag	UNP Q13085
D	-8	GLY	-	expression tag	UNP Q13085
D	-7	LEU	-	expression tag	UNP Q13085
D	-6	GLU	-	expression tag	UNP Q13085
D	-5	ASN	-	expression tag	UNP Q13085
D	-4	LEU	-	expression tag	UNP Q13085
D	-3	TYR	-	expression tag	UNP Q13085
D	-2	PHE	-	expression tag	UNP Q13085
D	-1	GLN	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP Q13085
E	-60	MET	-	initiating methionine	UNP Q13085
E	-59	ALA	-	expression tag	UNP Q13085
E	-58	HIS	-	expression tag	UNP Q13085
E	-57	HIS	-	expression tag	UNP Q13085
E	-56	HIS	-	expression tag	UNP Q13085
E	-55	HIS	-	expression tag	UNP Q13085
E	-54	HIS	-	expression tag	UNP Q13085
E	-53	HIS	-	expression tag	UNP Q13085
E	-52	HIS	-	expression tag	UNP Q13085
E	-51	HIS	-	expression tag	UNP Q13085
E	-50	HIS	-	expression tag	UNP Q13085
E	-49	HIS	-	expression tag	UNP Q13085
E	-48	GLY	-	expression tag	UNP Q13085
E	-47	SER	-	expression tag	UNP Q13085
E	-46	THR	-	expression tag	UNP Q13085
E	-45	SER	-	expression tag	UNP Q13085
E	-44	GLY	-	expression tag	UNP Q13085
E	-43	SER	-	expression tag	UNP Q13085
E	-42	GLY	-	expression tag	UNP Q13085
E	-41	GLU	-	expression tag	UNP Q13085
E	-40	GLN	-	expression tag	UNP Q13085
E	-39	LYS	-	expression tag	UNP Q13085
E	-38	LEU	-	expression tag	UNP Q13085
E	-37	ILE	-	expression tag	UNP Q13085
E	-36	SER	-	expression tag	UNP Q13085
E	-35	GLU	-	expression tag	UNP Q13085
E	-34	GLU	-	expression tag	UNP Q13085
E	-33	ASP	-	expression tag	UNP Q13085
E	-32	LEU	-	expression tag	UNP Q13085
E	-31	GLY	-	expression tag	UNP Q13085
E	-30	SER	-	expression tag	UNP Q13085
E	-29	THR	-	expression tag	UNP Q13085
E	-28	SER	-	expression tag	UNP Q13085
E	-27	GLY	-	expression tag	UNP Q13085
E	-26	SER	-	expression tag	UNP Q13085
E	-25	GLY	-	expression tag	UNP Q13085
E	-24	ASP	-	expression tag	UNP Q13085
E	-23	TYR	-	expression tag	UNP Q13085
E	-22	LYS	-	expression tag	UNP Q13085
E	-21	ASP	-	expression tag	UNP Q13085
E	-20	ASP	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	ASP	-	expression tag	UNP Q13085
E	-18	ASP	-	expression tag	UNP Q13085
E	-17	LYS	-	expression tag	UNP Q13085
E	-16	LEU	-	expression tag	UNP Q13085
E	-15	THR	-	expression tag	UNP Q13085
E	-14	SER	-	expression tag	UNP Q13085
E	-13	LEU	-	expression tag	UNP Q13085
E	-12	TYR	-	expression tag	UNP Q13085
E	-11	LYS	-	expression tag	UNP Q13085
E	-10	LYS	-	expression tag	UNP Q13085
E	-9	ALA	-	expression tag	UNP Q13085
E	-8	GLY	-	expression tag	UNP Q13085
E	-7	LEU	-	expression tag	UNP Q13085
E	-6	GLU	-	expression tag	UNP Q13085
E	-5	ASN	-	expression tag	UNP Q13085
E	-4	LEU	-	expression tag	UNP Q13085
E	-3	TYR	-	expression tag	UNP Q13085
E	-2	PHE	-	expression tag	UNP Q13085
E	-1	GLN	-	expression tag	UNP Q13085
E	0	GLY	-	expression tag	UNP Q13085
C	-60	MET	-	initiating methionine	UNP Q13085
C	-59	ALA	-	expression tag	UNP Q13085
C	-58	HIS	-	expression tag	UNP Q13085
C	-57	HIS	-	expression tag	UNP Q13085
C	-56	HIS	-	expression tag	UNP Q13085
C	-55	HIS	-	expression tag	UNP Q13085
C	-54	HIS	-	expression tag	UNP Q13085
C	-53	HIS	-	expression tag	UNP Q13085
C	-52	HIS	-	expression tag	UNP Q13085
C	-51	HIS	-	expression tag	UNP Q13085
C	-50	HIS	-	expression tag	UNP Q13085
C	-49	HIS	-	expression tag	UNP Q13085
C	-48	GLY	-	expression tag	UNP Q13085
C	-47	SER	-	expression tag	UNP Q13085
C	-46	THR	-	expression tag	UNP Q13085
C	-45	SER	-	expression tag	UNP Q13085
C	-44	GLY	-	expression tag	UNP Q13085
C	-43	SER	-	expression tag	UNP Q13085
C	-42	GLY	-	expression tag	UNP Q13085
C	-41	GLU	-	expression tag	UNP Q13085
C	-40	GLN	-	expression tag	UNP Q13085
C	-39	LYS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-38	LEU	-	expression tag	UNP Q13085
C	-37	ILE	-	expression tag	UNP Q13085
C	-36	SER	-	expression tag	UNP Q13085
C	-35	GLU	-	expression tag	UNP Q13085
C	-34	GLU	-	expression tag	UNP Q13085
C	-33	ASP	-	expression tag	UNP Q13085
C	-32	LEU	-	expression tag	UNP Q13085
C	-31	GLY	-	expression tag	UNP Q13085
C	-30	SER	-	expression tag	UNP Q13085
C	-29	THR	-	expression tag	UNP Q13085
C	-28	SER	-	expression tag	UNP Q13085
C	-27	GLY	-	expression tag	UNP Q13085
C	-26	SER	-	expression tag	UNP Q13085
C	-25	GLY	-	expression tag	UNP Q13085
C	-24	ASP	-	expression tag	UNP Q13085
C	-23	TYR	-	expression tag	UNP Q13085
C	-22	LYS	-	expression tag	UNP Q13085
C	-21	ASP	-	expression tag	UNP Q13085
C	-20	ASP	-	expression tag	UNP Q13085
C	-19	ASP	-	expression tag	UNP Q13085
C	-18	ASP	-	expression tag	UNP Q13085
C	-17	LYS	-	expression tag	UNP Q13085
C	-16	LEU	-	expression tag	UNP Q13085
C	-15	THR	-	expression tag	UNP Q13085
C	-14	SER	-	expression tag	UNP Q13085
C	-13	LEU	-	expression tag	UNP Q13085
C	-12	TYR	-	expression tag	UNP Q13085
C	-11	LYS	-	expression tag	UNP Q13085
C	-10	LYS	-	expression tag	UNP Q13085
C	-9	ALA	-	expression tag	UNP Q13085
C	-8	GLY	-	expression tag	UNP Q13085
C	-7	LEU	-	expression tag	UNP Q13085
C	-6	GLU	-	expression tag	UNP Q13085
C	-5	ASN	-	expression tag	UNP Q13085
C	-4	LEU	-	expression tag	UNP Q13085
C	-3	TYR	-	expression tag	UNP Q13085
C	-2	PHE	-	expression tag	UNP Q13085
C	-1	GLN	-	expression tag	UNP Q13085
C	0	GLY	-	expression tag	UNP Q13085
F	-60	MET	-	initiating methionine	UNP Q13085
F	-59	ALA	-	expression tag	UNP Q13085
F	-58	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-57	HIS	-	expression tag	UNP Q13085
F	-56	HIS	-	expression tag	UNP Q13085
F	-55	HIS	-	expression tag	UNP Q13085
F	-54	HIS	-	expression tag	UNP Q13085
F	-53	HIS	-	expression tag	UNP Q13085
F	-52	HIS	-	expression tag	UNP Q13085
F	-51	HIS	-	expression tag	UNP Q13085
F	-50	HIS	-	expression tag	UNP Q13085
F	-49	HIS	-	expression tag	UNP Q13085
F	-48	GLY	-	expression tag	UNP Q13085
F	-47	SER	-	expression tag	UNP Q13085
F	-46	THR	-	expression tag	UNP Q13085
F	-45	SER	-	expression tag	UNP Q13085
F	-44	GLY	-	expression tag	UNP Q13085
F	-43	SER	-	expression tag	UNP Q13085
F	-42	GLY	-	expression tag	UNP Q13085
F	-41	GLU	-	expression tag	UNP Q13085
F	-40	GLN	-	expression tag	UNP Q13085
F	-39	LYS	-	expression tag	UNP Q13085
F	-38	LEU	-	expression tag	UNP Q13085
F	-37	ILE	-	expression tag	UNP Q13085
F	-36	SER	-	expression tag	UNP Q13085
F	-35	GLU	-	expression tag	UNP Q13085
F	-34	GLU	-	expression tag	UNP Q13085
F	-33	ASP	-	expression tag	UNP Q13085
F	-32	LEU	-	expression tag	UNP Q13085
F	-31	GLY	-	expression tag	UNP Q13085
F	-30	SER	-	expression tag	UNP Q13085
F	-29	THR	-	expression tag	UNP Q13085
F	-28	SER	-	expression tag	UNP Q13085
F	-27	GLY	-	expression tag	UNP Q13085
F	-26	SER	-	expression tag	UNP Q13085
F	-25	GLY	-	expression tag	UNP Q13085
F	-24	ASP	-	expression tag	UNP Q13085
F	-23	TYR	-	expression tag	UNP Q13085
F	-22	LYS	-	expression tag	UNP Q13085
F	-21	ASP	-	expression tag	UNP Q13085
F	-20	ASP	-	expression tag	UNP Q13085
F	-19	ASP	-	expression tag	UNP Q13085
F	-18	ASP	-	expression tag	UNP Q13085
F	-17	LYS	-	expression tag	UNP Q13085
F	-16	LEU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	THR	-	expression tag	UNP Q13085
F	-14	SER	-	expression tag	UNP Q13085
F	-13	LEU	-	expression tag	UNP Q13085
F	-12	TYR	-	expression tag	UNP Q13085
F	-11	LYS	-	expression tag	UNP Q13085
F	-10	LYS	-	expression tag	UNP Q13085
F	-9	ALA	-	expression tag	UNP Q13085
F	-8	GLY	-	expression tag	UNP Q13085
F	-7	LEU	-	expression tag	UNP Q13085
F	-6	GLU	-	expression tag	UNP Q13085
F	-5	ASN	-	expression tag	UNP Q13085
F	-4	LEU	-	expression tag	UNP Q13085
F	-3	TYR	-	expression tag	UNP Q13085
F	-2	PHE	-	expression tag	UNP Q13085
F	-1	GLN	-	expression tag	UNP Q13085
F	0	GLY	-	expression tag	UNP Q13085
B	-60	MET	-	initiating methionine	UNP Q13085
B	-59	ALA	-	expression tag	UNP Q13085
B	-58	HIS	-	expression tag	UNP Q13085
B	-57	HIS	-	expression tag	UNP Q13085
B	-56	HIS	-	expression tag	UNP Q13085
B	-55	HIS	-	expression tag	UNP Q13085
B	-54	HIS	-	expression tag	UNP Q13085
B	-53	HIS	-	expression tag	UNP Q13085
B	-52	HIS	-	expression tag	UNP Q13085
B	-51	HIS	-	expression tag	UNP Q13085
B	-50	HIS	-	expression tag	UNP Q13085
B	-49	HIS	-	expression tag	UNP Q13085
B	-48	GLY	-	expression tag	UNP Q13085
B	-47	SER	-	expression tag	UNP Q13085
B	-46	THR	-	expression tag	UNP Q13085
B	-45	SER	-	expression tag	UNP Q13085
B	-44	GLY	-	expression tag	UNP Q13085
B	-43	SER	-	expression tag	UNP Q13085
B	-42	GLY	-	expression tag	UNP Q13085
B	-41	GLU	-	expression tag	UNP Q13085
B	-40	GLN	-	expression tag	UNP Q13085
B	-39	LYS	-	expression tag	UNP Q13085
B	-38	LEU	-	expression tag	UNP Q13085
B	-37	ILE	-	expression tag	UNP Q13085
B	-36	SER	-	expression tag	UNP Q13085
B	-35	GLU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	GLU	-	expression tag	UNP Q13085
B	-33	ASP	-	expression tag	UNP Q13085
B	-32	LEU	-	expression tag	UNP Q13085
B	-31	GLY	-	expression tag	UNP Q13085
B	-30	SER	-	expression tag	UNP Q13085
B	-29	THR	-	expression tag	UNP Q13085
B	-28	SER	-	expression tag	UNP Q13085
B	-27	GLY	-	expression tag	UNP Q13085
B	-26	SER	-	expression tag	UNP Q13085
B	-25	GLY	-	expression tag	UNP Q13085
B	-24	ASP	-	expression tag	UNP Q13085
B	-23	TYR	-	expression tag	UNP Q13085
B	-22	LYS	-	expression tag	UNP Q13085
B	-21	ASP	-	expression tag	UNP Q13085
B	-20	ASP	-	expression tag	UNP Q13085
B	-19	ASP	-	expression tag	UNP Q13085
B	-18	ASP	-	expression tag	UNP Q13085
B	-17	LYS	-	expression tag	UNP Q13085
B	-16	LEU	-	expression tag	UNP Q13085
B	-15	THR	-	expression tag	UNP Q13085
B	-14	SER	-	expression tag	UNP Q13085
B	-13	LEU	-	expression tag	UNP Q13085
B	-12	TYR	-	expression tag	UNP Q13085
B	-11	LYS	-	expression tag	UNP Q13085
B	-10	LYS	-	expression tag	UNP Q13085
B	-9	ALA	-	expression tag	UNP Q13085
B	-8	GLY	-	expression tag	UNP Q13085
B	-7	LEU	-	expression tag	UNP Q13085
B	-6	GLU	-	expression tag	UNP Q13085
B	-5	ASN	-	expression tag	UNP Q13085
B	-4	LEU	-	expression tag	UNP Q13085
B	-3	TYR	-	expression tag	UNP Q13085
B	-2	PHE	-	expression tag	UNP Q13085
B	-1	GLN	-	expression tag	UNP Q13085
B	0	GLY	-	expression tag	UNP Q13085
A	-60	MET	-	initiating methionine	UNP Q13085
A	-59	ALA	-	expression tag	UNP Q13085
A	-58	HIS	-	expression tag	UNP Q13085
A	-57	HIS	-	expression tag	UNP Q13085
A	-56	HIS	-	expression tag	UNP Q13085
A	-55	HIS	-	expression tag	UNP Q13085
A	-54	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-53	HIS	-	expression tag	UNP Q13085
A	-52	HIS	-	expression tag	UNP Q13085
A	-51	HIS	-	expression tag	UNP Q13085
A	-50	HIS	-	expression tag	UNP Q13085
A	-49	HIS	-	expression tag	UNP Q13085
A	-48	GLY	-	expression tag	UNP Q13085
A	-47	SER	-	expression tag	UNP Q13085
A	-46	THR	-	expression tag	UNP Q13085
A	-45	SER	-	expression tag	UNP Q13085
A	-44	GLY	-	expression tag	UNP Q13085
A	-43	SER	-	expression tag	UNP Q13085
A	-42	GLY	-	expression tag	UNP Q13085
A	-41	GLU	-	expression tag	UNP Q13085
A	-40	GLN	-	expression tag	UNP Q13085
A	-39	LYS	-	expression tag	UNP Q13085
A	-38	LEU	-	expression tag	UNP Q13085
A	-37	ILE	-	expression tag	UNP Q13085
A	-36	SER	-	expression tag	UNP Q13085
A	-35	GLU	-	expression tag	UNP Q13085
A	-34	GLU	-	expression tag	UNP Q13085
A	-33	ASP	-	expression tag	UNP Q13085
A	-32	LEU	-	expression tag	UNP Q13085
A	-31	GLY	-	expression tag	UNP Q13085
A	-30	SER	-	expression tag	UNP Q13085
A	-29	THR	-	expression tag	UNP Q13085
A	-28	SER	-	expression tag	UNP Q13085
A	-27	GLY	-	expression tag	UNP Q13085
A	-26	SER	-	expression tag	UNP Q13085
A	-25	GLY	-	expression tag	UNP Q13085
A	-24	ASP	-	expression tag	UNP Q13085
A	-23	TYR	-	expression tag	UNP Q13085
A	-22	LYS	-	expression tag	UNP Q13085
A	-21	ASP	-	expression tag	UNP Q13085
A	-20	ASP	-	expression tag	UNP Q13085
A	-19	ASP	-	expression tag	UNP Q13085
A	-18	ASP	-	expression tag	UNP Q13085
A	-17	LYS	-	expression tag	UNP Q13085
A	-16	LEU	-	expression tag	UNP Q13085
A	-15	THR	-	expression tag	UNP Q13085
A	-14	SER	-	expression tag	UNP Q13085
A	-13	LEU	-	expression tag	UNP Q13085
A	-12	TYR	-	expression tag	UNP Q13085

Continued on next page...

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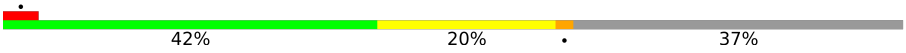
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	LYS	-	expression tag	UNP Q13085
A	-10	LYS	-	expression tag	UNP Q13085
A	-9	ALA	-	expression tag	UNP Q13085
A	-8	GLY	-	expression tag	UNP Q13085
A	-7	LEU	-	expression tag	UNP Q13085
A	-6	GLU	-	expression tag	UNP Q13085
A	-5	ASN	-	expression tag	UNP Q13085
A	-4	LEU	-	expression tag	UNP Q13085
A	-3	TYR	-	expression tag	UNP Q13085
A	-2	PHE	-	expression tag	UNP Q13085
A	-1	GLN	-	expression tag	UNP Q13085
A	0	GLY	-	expression tag	UNP Q13085

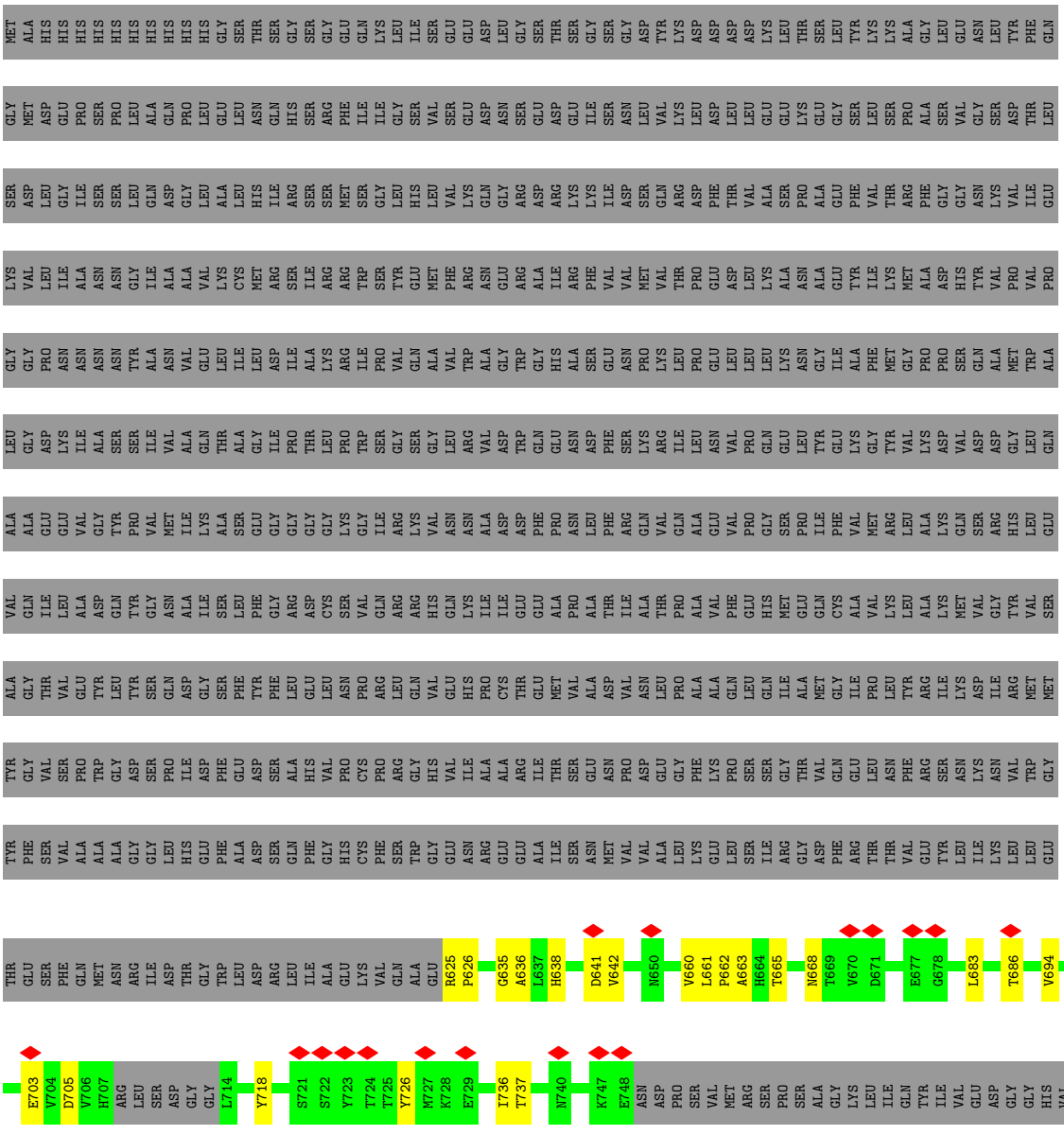
3 Residue-property plots (i)

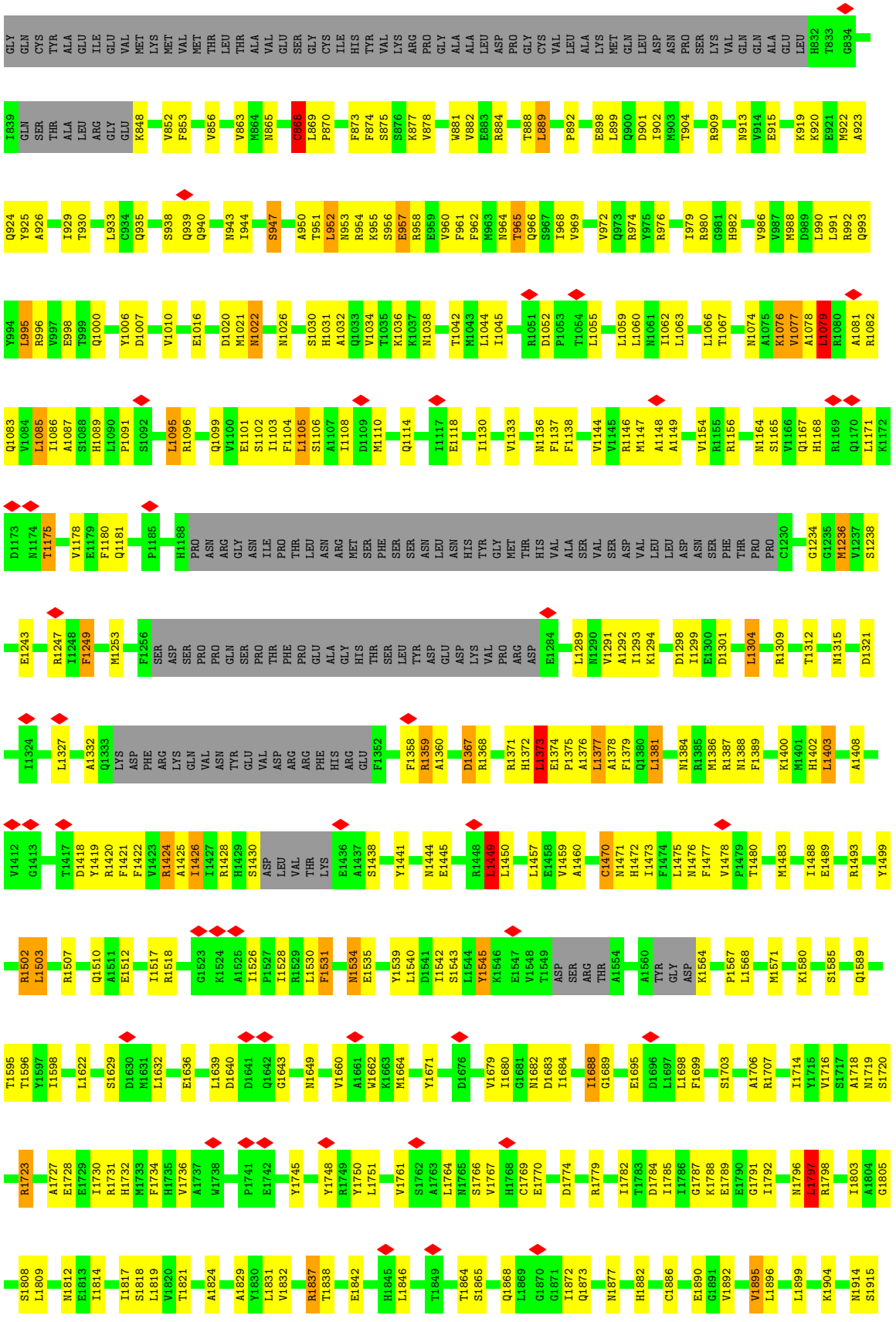
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

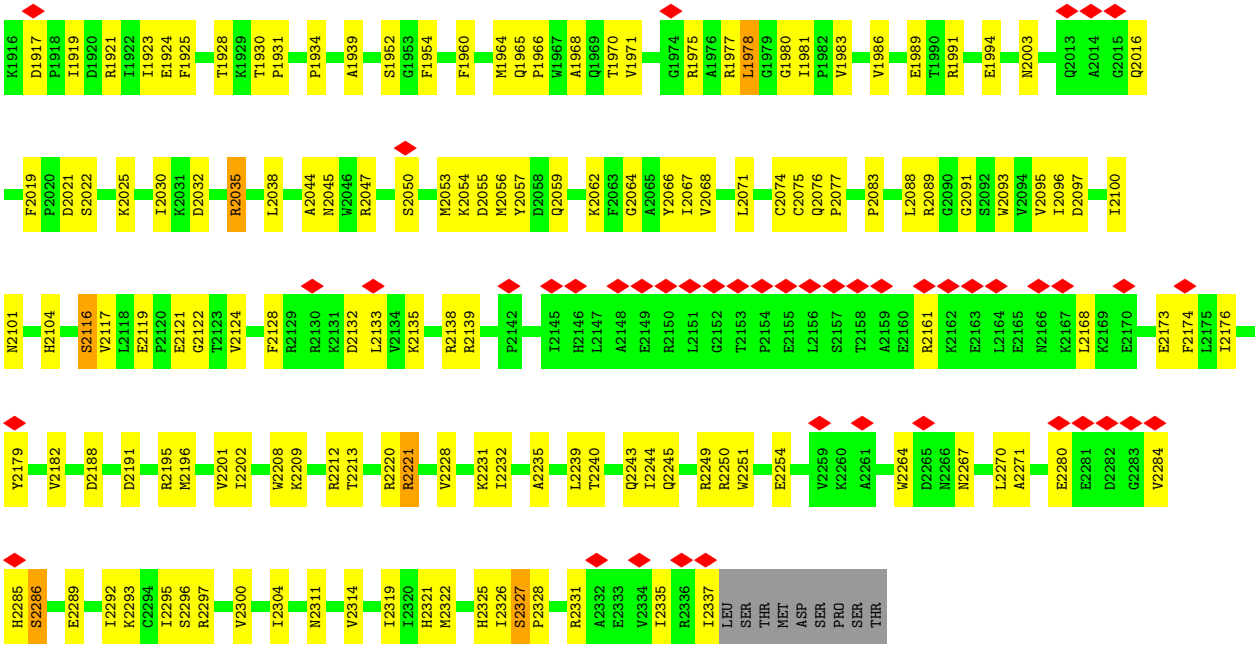
- Molecule 1: Acetyl-CoA carboxylase 1

Chain D:



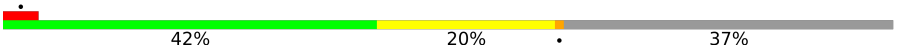


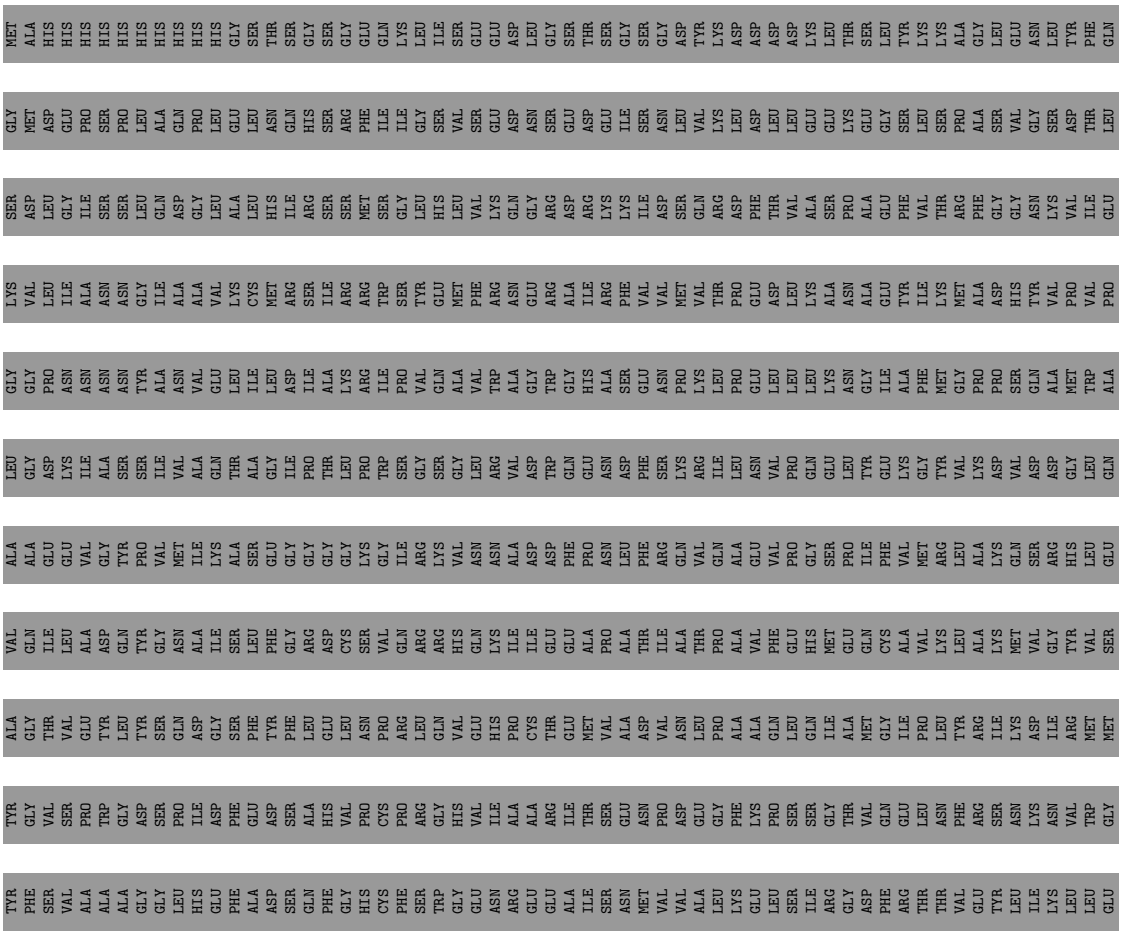


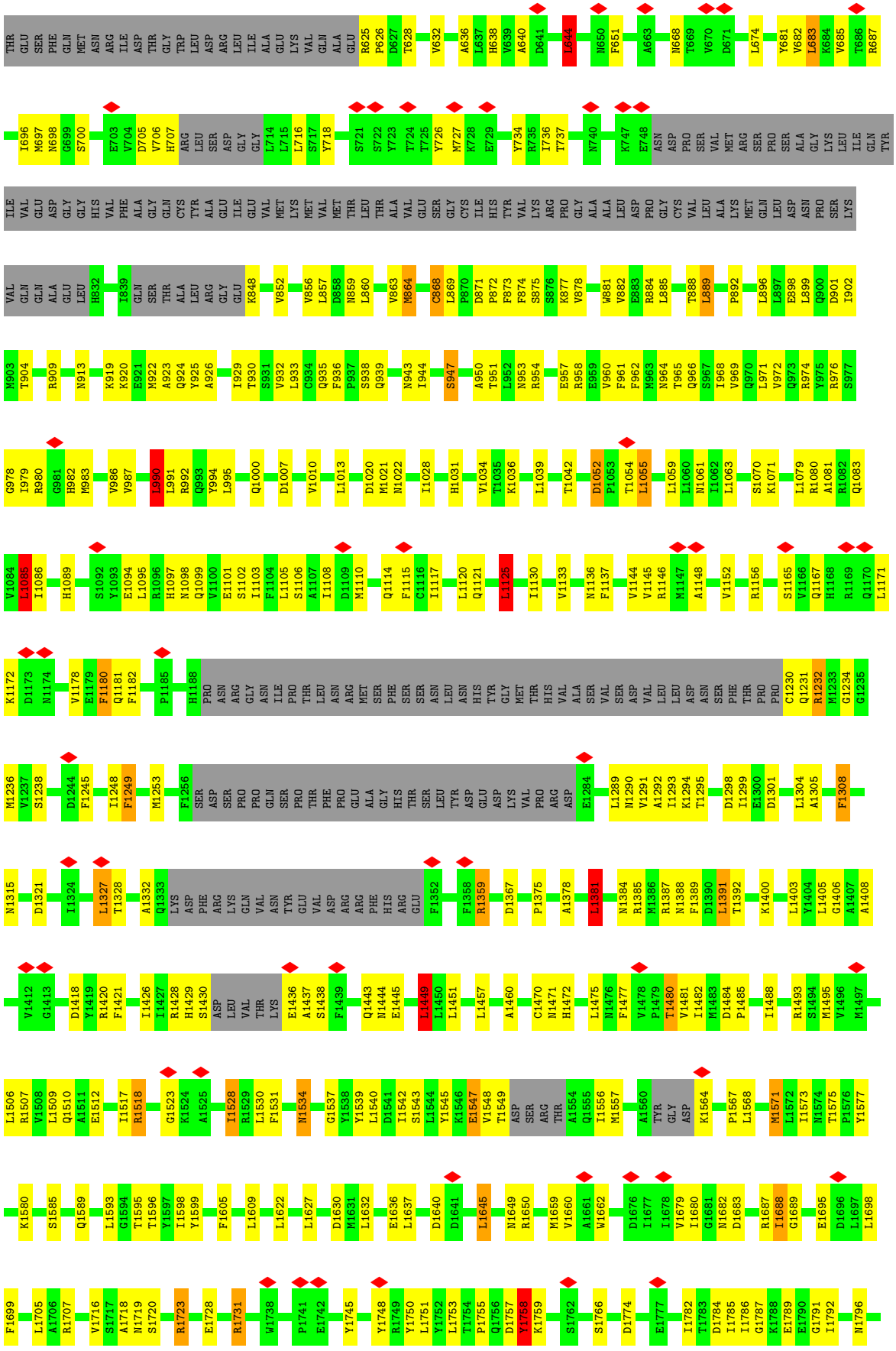


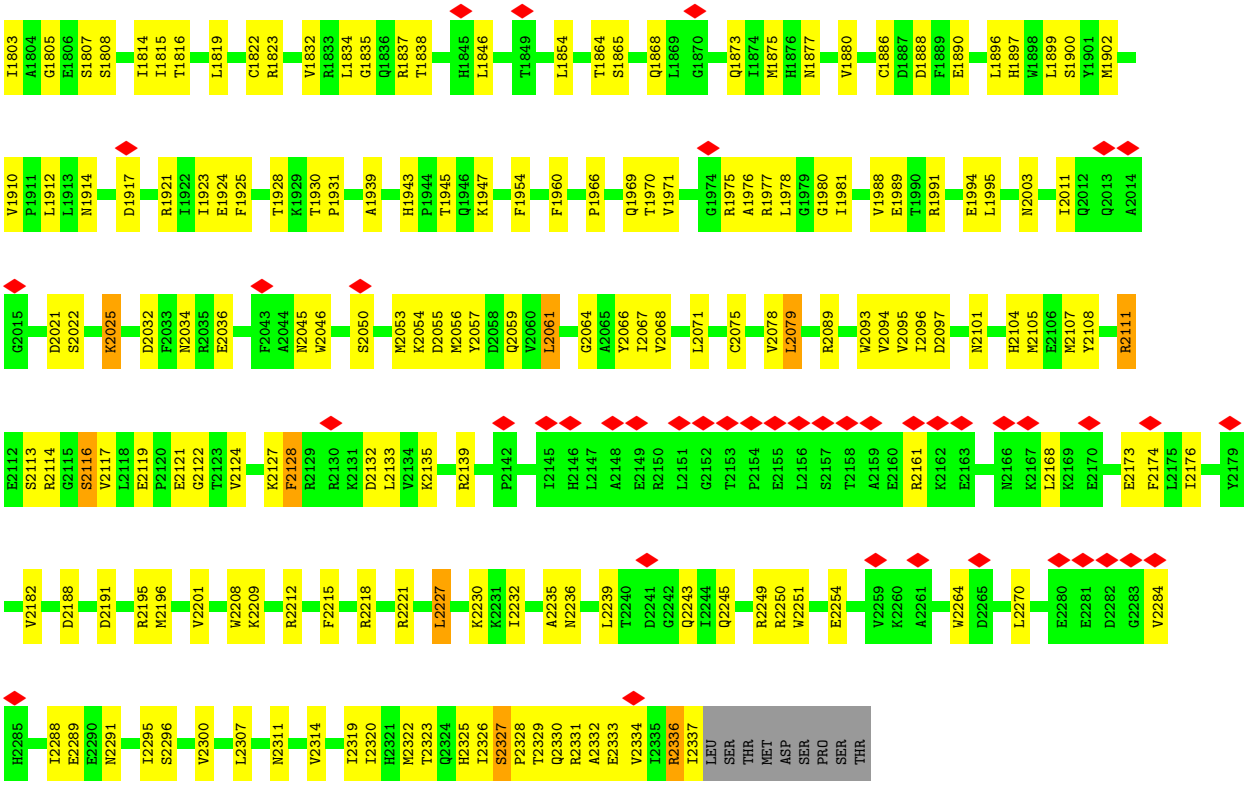
- Molecule 1: Acetyl-CoA carboxylase 1

Chain E:



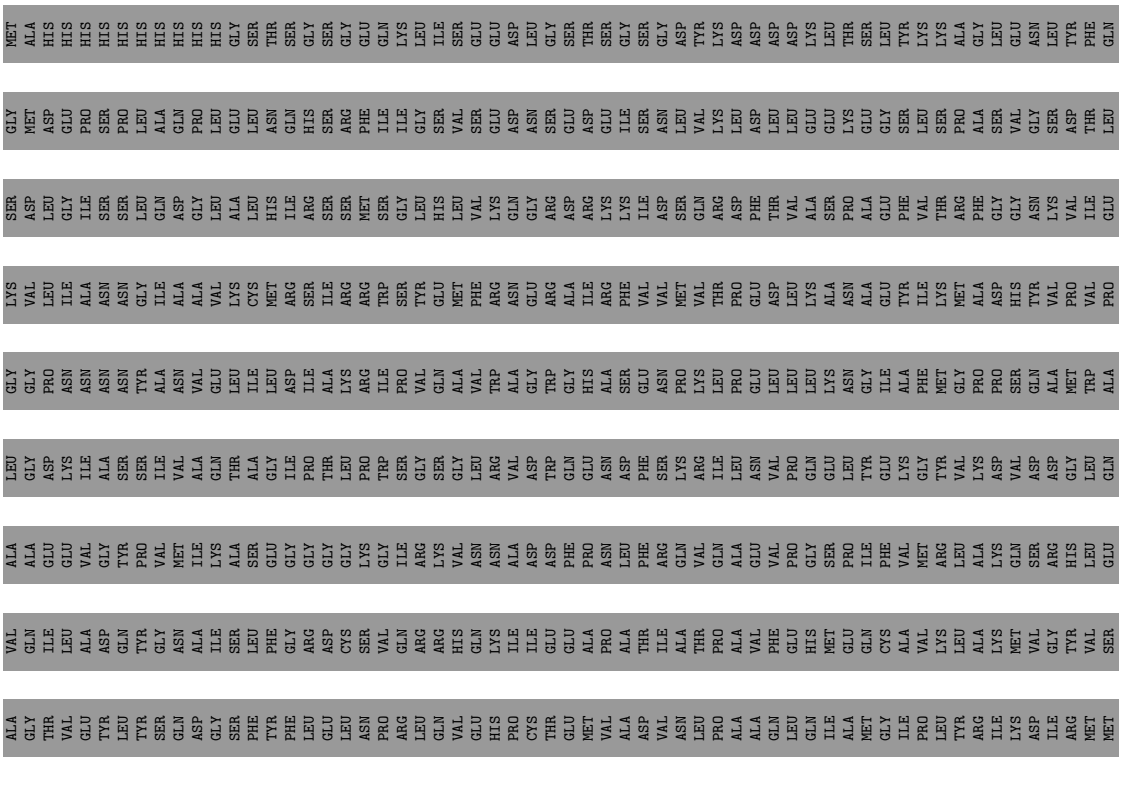


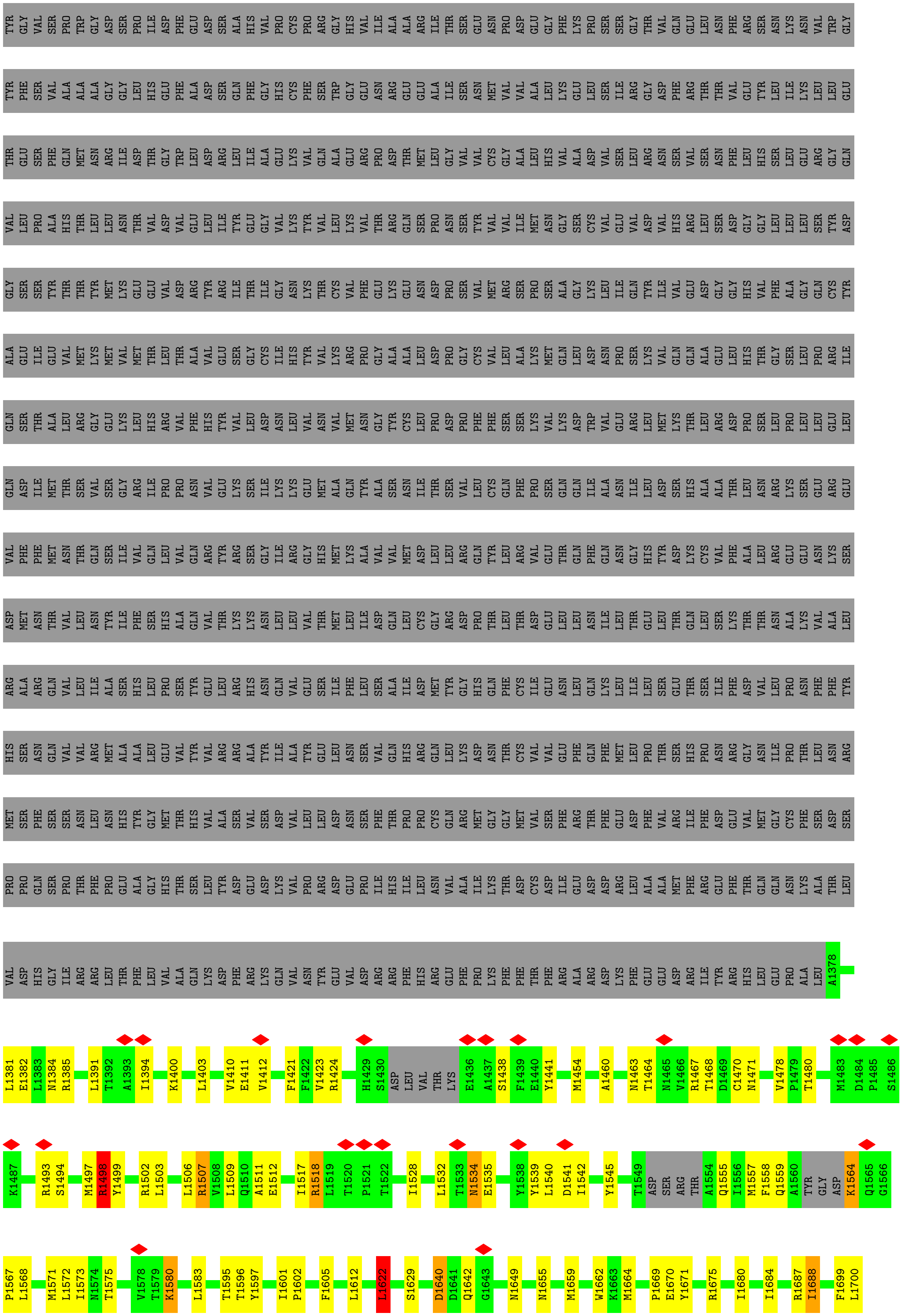




• Molecule 1: Acetyl-CoA carboxylase 1

Chain C:

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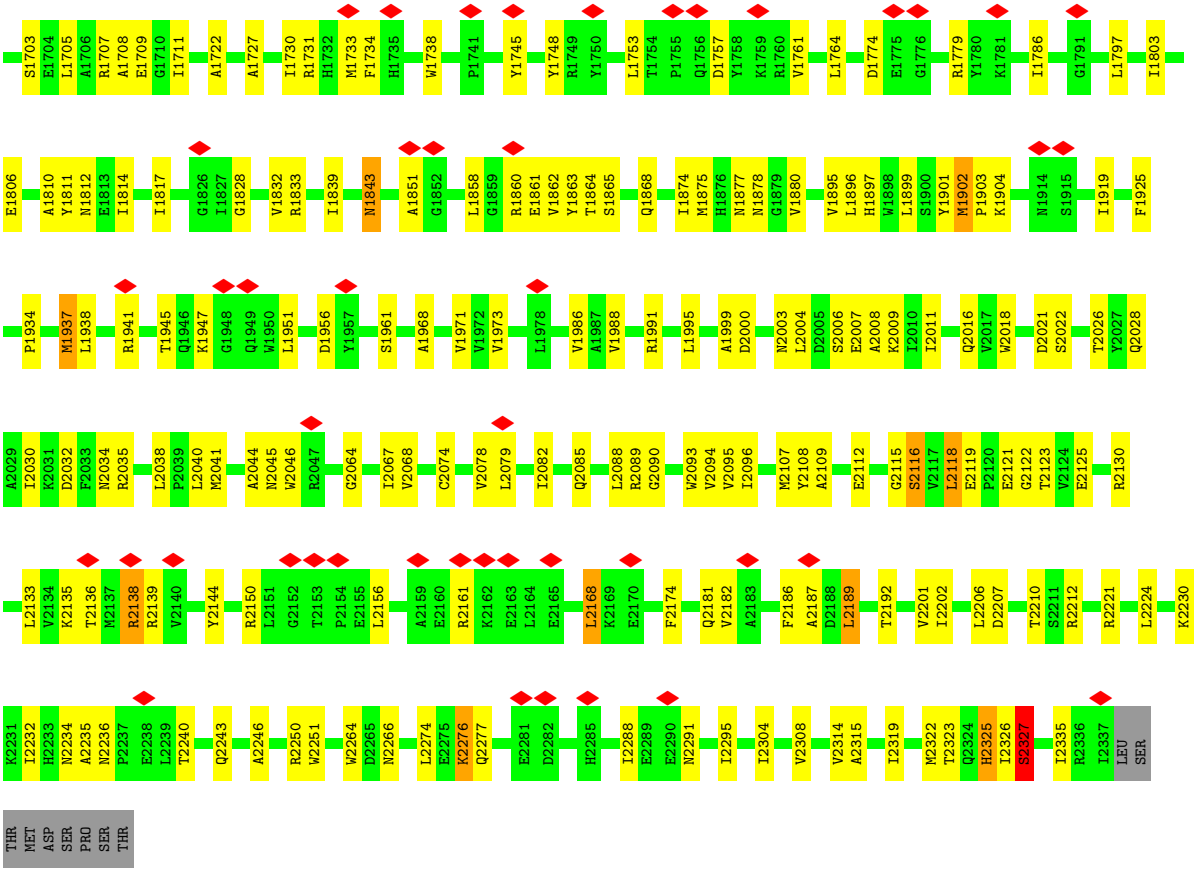
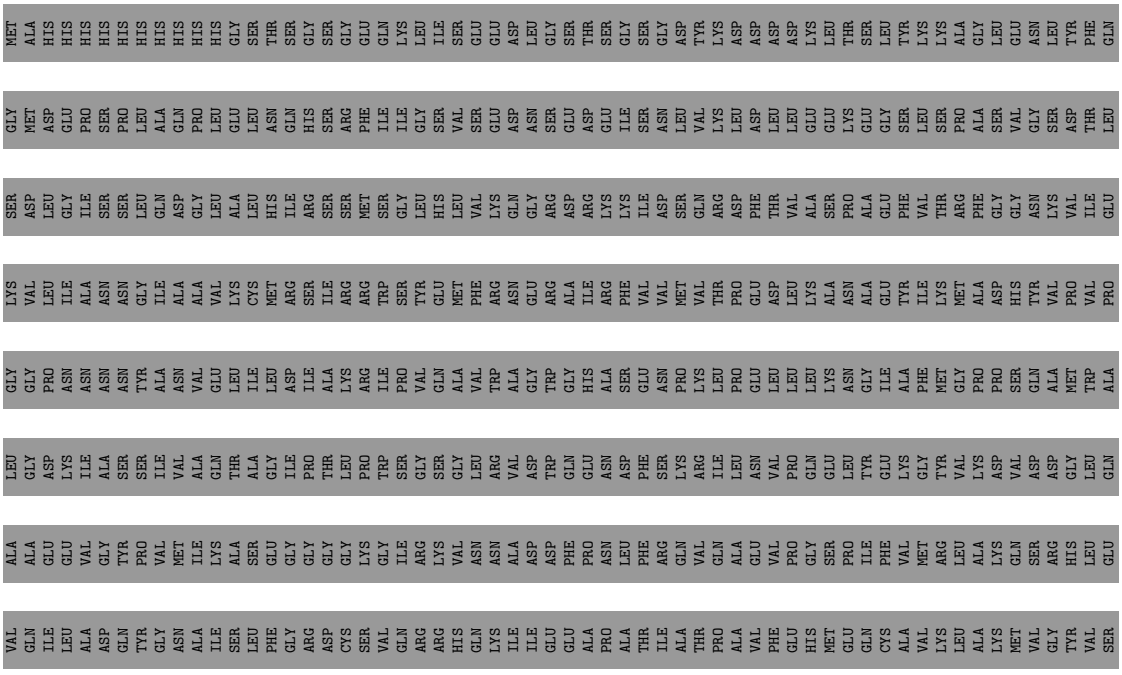
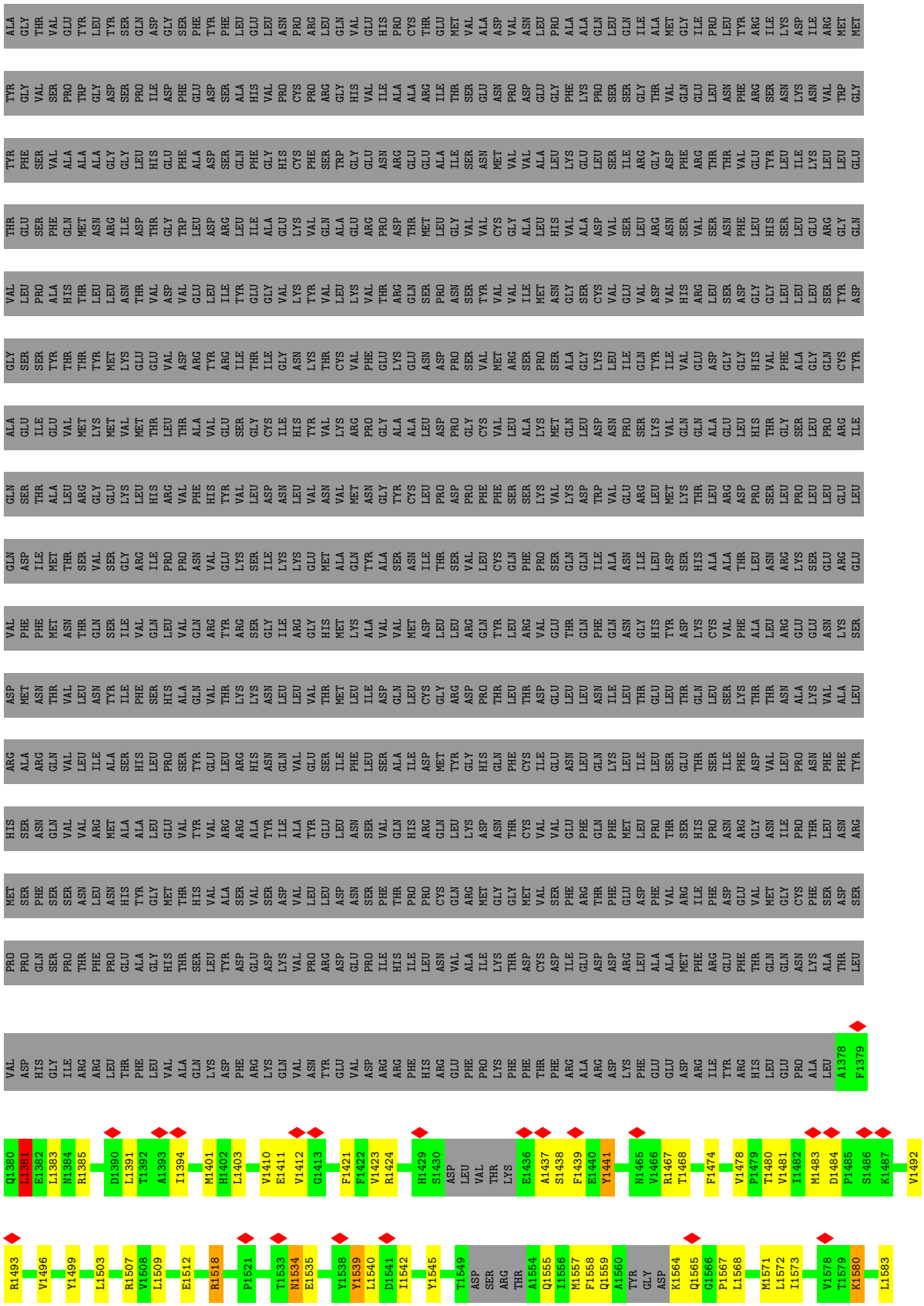
TYR PHE SER VAL ALA ALA ALA GLY GLY LEU HIS GLU PHE ALA ASP SER GLN PHE GLY HIS CYS PHE SER TRP GLY GLU ASN ARG GLU GLU ALA ILE SER ASN MET VAL VAL ALA LEU LYS GLU LEU SER ILE ARG GLY ASP PHE ARG THR THR VAL GLU TYR LEU ILE LYS LEU LEU GLU
THR GLU SER PHE GLN MET ASN ARG ILE ASP THR GLY TRP LEU ASP ARG LEU ILE ALA GLU LYS VAL GLN ALA GLU ARG PRO ASP THR MET LEU GLY VAL VAL CYS GLY ALA LEU HIS VAL ALA ASP VAL SER LEU ARG ASN SER VAL SER ASN PHE LEU HIS SER LEU GLU ARG GLY GLN
VAL LEU PRO ALA HIS THR LEU LEU ASN THR VAL ASP VAL GLU LEU ILE TYR GLU GLY VAL LYS TYR VAL LEU LYS VAL THR ARG GLN SER PRO ASN SER TYR VAL VAL ILE MET ASN GLY SER CYS VAL GLU VAL ASP VAL HIS ARG LEU SER ASP GLY GLY LEU LEU LEU SER TYR ASP
GLY SER SER TYR THR THR TYR MET LYS GLU GLU VAL ASP ARG TYR ARG ILE THR ILE GLY ASN LYS THR CYS VAL PHE GLU LYS GLU ASN ASP PRO SER VAL MET ARG SER PRO SER ALA GLY LYS LEU ILE GLN TYR ILE VAL GLU ASP GLY GLY HIS VAL PHE ALA GLY GLN CYS TYR
ALA GLU ILE GLU VAL MET LYS MET VAL MET THR LEU THR ALA VAL GLU SER GLY CYS ILE HIS TYR VAL LYS ARG PRO GLY ALA ALA LEU ASP PRO GLY CYS VAL LEU ALA LYS MET GLN LEU ASP ASN PRO SER LYS VAL GLN GLN ALA GLU LEU HIS THR GLY SER LEU PRO ARG ILE
GLN SER THR ALA LEU ARG GLY GLU LYS LEU HIS ARG VAL PHE HIS TYR VAL LEU ASP ASN LEU VAL ASN VAL MET ASN GLY TYR CYS LEU PRO ASP PRO PHE PHE SER SER LYS VAL LYS ASP TRP VAL GLU ARG LEU MET LYS THR LEU ARG ASP PRO SER LEU PRO LEU LEU GLU LEU
GLN ASP ILE MET THR SER VAL SER GLY ARG ILE PRO PRO ASN VAL GLU LYS SER ILE LYS LYS GLU MET ALA GLN TYR ALA SER ASN ILE THR SER VAL LEU CYS GLN PHE PRO SER GLN GLN ILE ALA ASN ILE LEU ASP SER HIS ALA ALA THR LEU ASN ARG LYS SER GLU ARG GLU
VAL PHE PHE MET ASN THR GLN SER ILE VAL GLN LEU VAL GLN ARG TYR ARG SER GLY ILE ARG GLY HIS MET LYS ALA VAL VAL MET ASP LEU LEU ARG GLN TYR LEU ARG VAL GLU THR GLN PHE GLN ASN GLY HIS TYR ASP LYS CYS VAL PHE ALA LEU ARG GLU GLU ASN LYS SER
ASP MET ASN THR VAL LEU ASN TYR ILE PHE SER HIS ALA GLN VAL THR LYS LYS ASN LEU LEU VAL THR MET LEU ILE ASP GLN LEU CYS GLY ARG ASP PRO THR LEU THR ASP GLU LEU LEU ASN ILE LEU THR GLU LEU THR GLN LEU SER LYS THR THR ASN ALA LYS VAL ALA LEU
ARG ALA ARG GLN VAL LEU ILE ALA SER HIS LEU PRO SER TYR GLU LEU ARG HIS ASN GLN VAL GLU SER ILE PHE LEU SER ALA ILE ASP MET TYR GLY HIS GLN PHE CYS ILE GLU ASN LEU GLN LYS LEU ILE LEU SER GLU THR SER ILE PHE ASP VAL LEU PRO ASN PHE PHE TYR
HIS SER ASN GLN VAL VAL ARG MET ALA ALA LEU GLU VAL TYR VAL ARG ARG ALA TYR ILE ALA TYR GLU LEU ASN SER VAL GLN HIS ARG GLN LEU LYS ASP ASN THR CYS VAL VAL GLU PHE GLN PHE MET LEU PRO THR SER HIS PRO ASN ARG GLY ASN ILE PRO THR LEU ASN ARG
MET SER PHE SER SER ASN LEU ASN HIS TYR GLY MET THR HIS VAL ALA SER VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO CYS GLN ARG MET GLY GLY MET VAL SER PHE ARG THR PHE GLU ASP PHE VAL ARG ILE PHE ASP GLU VAL MET GLY CYS PHE SER ASP SER
PRO PRO GLN SER PRO THR PHE PRO GLU ALA GLY HIS THR SER LEU TYR ASP GLU ASP LYS VAL PRO ARG ASP GLU PRO ILE HIS ILE LEU ASN VAL ALA ILE LYS THR ASP CYS ASP ILE GLU ASP ASP ARG LEU ALA ALA MET PHE ARG GLU PHE THR GLN GLN ASN LYS ALA THR LEU
VAL ASP HIS GLY ILE ARG ARG LEU THR PHE LEU VAL ALA GLN LYS ASP PHE ARG LYS GLN VAL ASN TYR GLU VAL ASP ARG ARG PHE HIS ARG GLU PHE PRO LYS PHE PHE THR PHE ARG ALA ARG ASP LYS PHE GLU GLU ASP ARG ILE TYR ARG HIS LEU GLU PRO ALA LEU A1378
L1381 E1382 L1383 N1384 R1385 L1391 T1392 A1393 I1394 K1400 L1403 V1410 E1411 V1412 F1421 F1422 V1423 R1424 H1429 S1430 ASP LEU VAL THR LYS E1436 A1437 S1438 F1439 E1440 Y1441 M1454 A1460 N1463 T1464 N1465 V1466 R1467 T1468 D1469 C1470 N1471 V1478 P1479 T1480 M1483 D1484 P1485 S1486
K1487 R1493 S1494 M1497 R1498 Y1499 R1502 L1503 L1506 R1507 V1508 L1509 Q1510 A1511 E1512 I1517 R1518 L1519 T1520 P1521 T1522 I1528 L1532 T1533 N1534 E1535 Y1538 Y1539 L1540 D1541 I1542 Y1545 T1549 ASP SER ARG THR A1554 Q1555 I1556 M1557 F1558 Q1559 A1560 TYR GLY ASP K1564 Q1565 G1566
P1567 L1568 M1571 L1572 I1573 N1574 T1575 V1578 T1579 K1580 L1583 T1595 T1596 Y1597 I1601 P1602 F1605 L1612 L1622 S1629 D1640 D1641 Q1642 G1643 N1649 N1655 M1659 W1662 K1663 M1664 P1669 E1670 Y1671 R1675 I1680 I1684 R1687 I1688 F1699 L1700

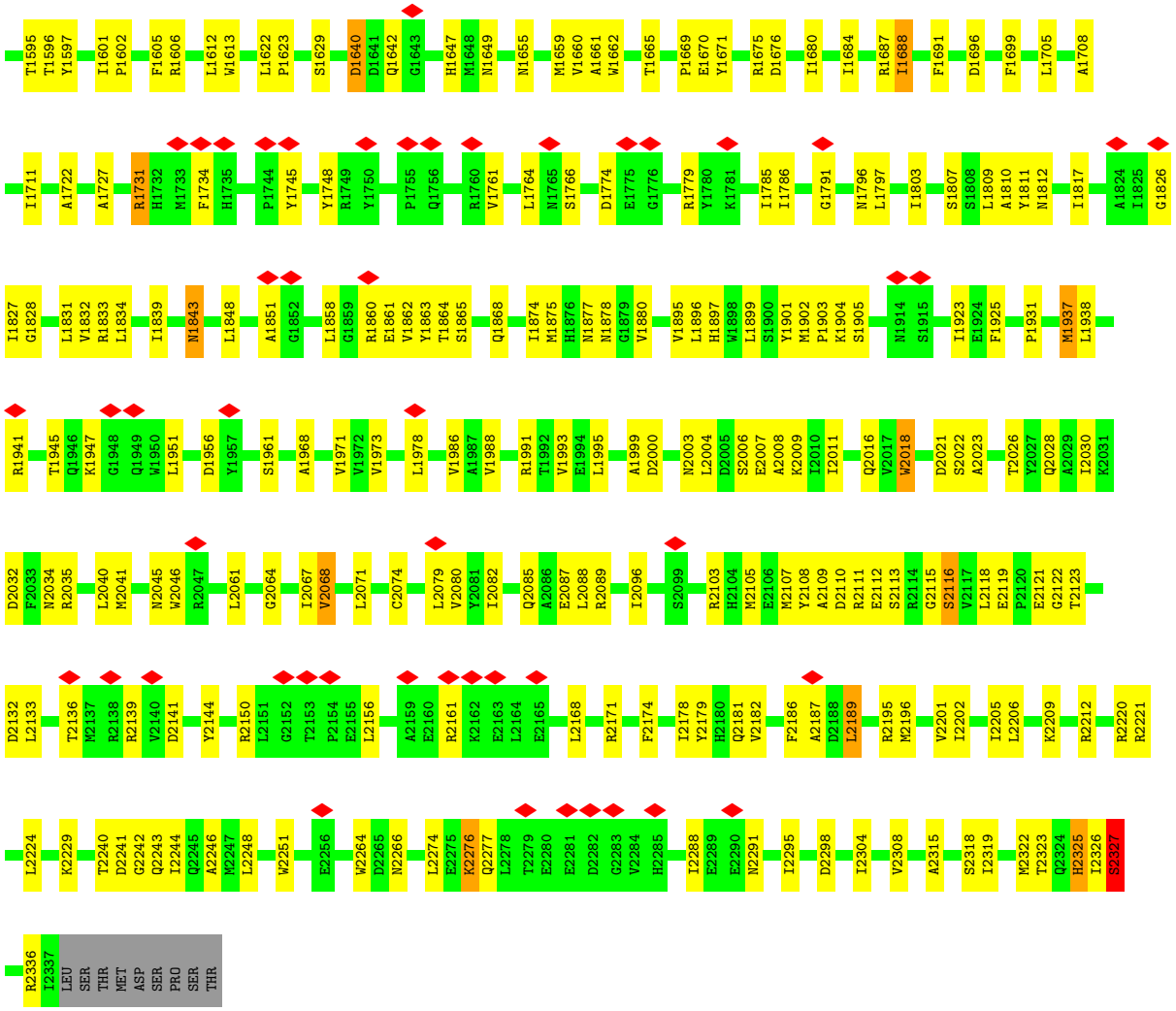


- Molecule 1: Acetyl-CoA carboxylase 1

Chain F:

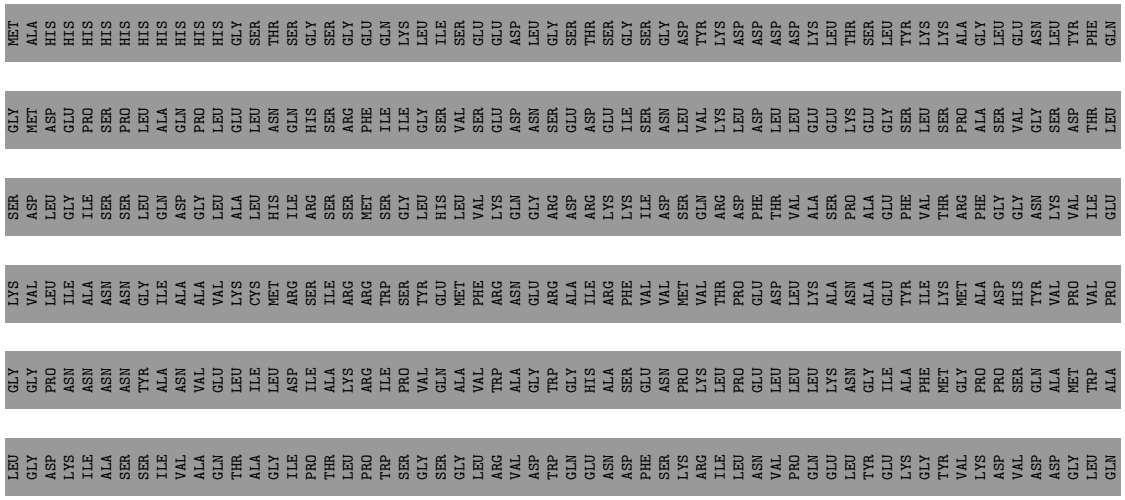


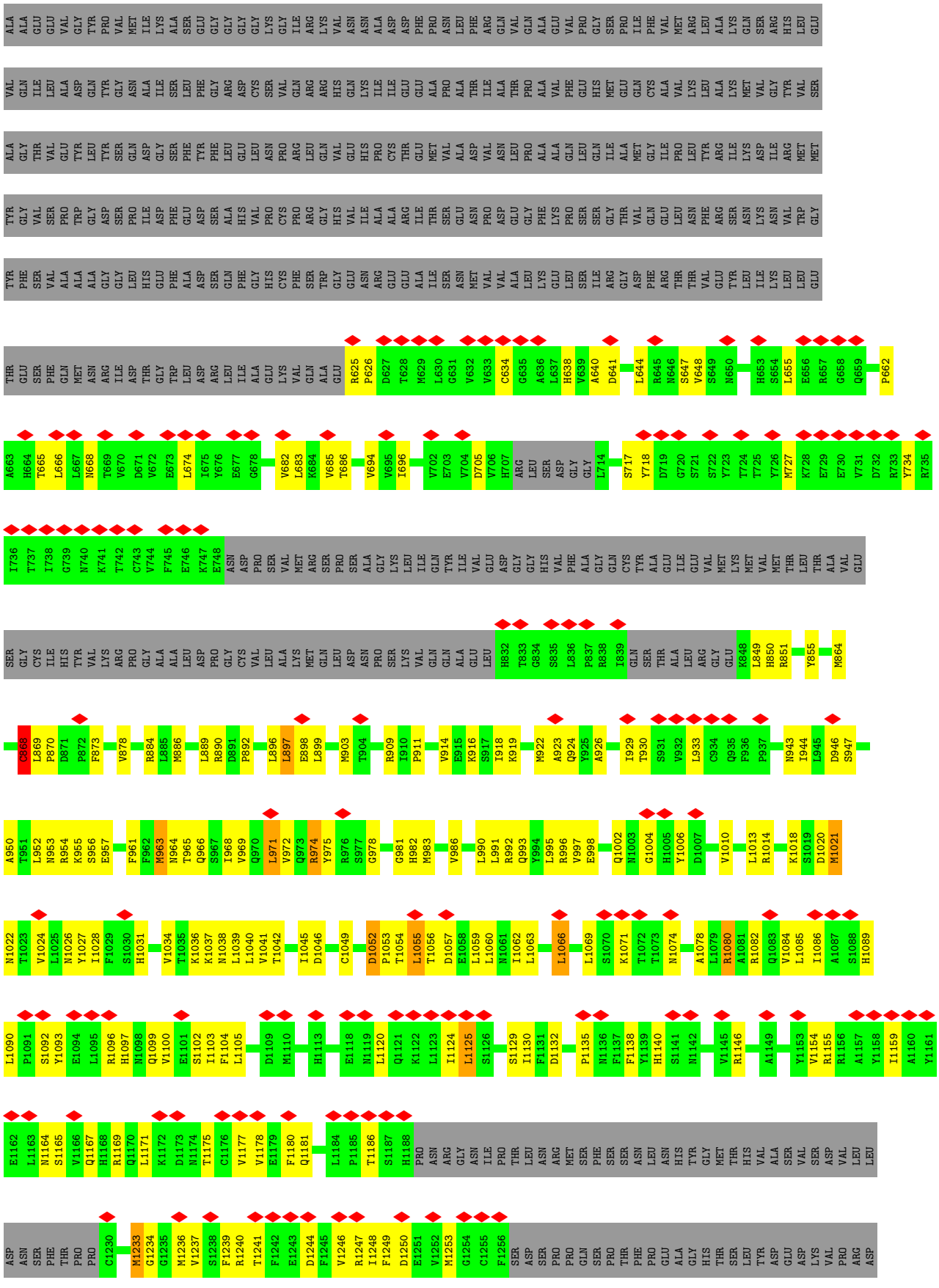

Q1380 L1381 E1382 L1383 N1384 R1385 D1390 L1391 T1392 A1393 I1394 M1401 H1402 L1403 V1410 E1411 V1412 G1413 F1421 F1422 V1423 R1424 H1429 S1430 ASP LEU VAL THR LYS E1436 A1437 S1438 F1439 E1440 Y1441 N1465 V1466 R1467 T1468 F1474 V1478 P1479 T1480 V1481 I1482 M1483 D1484 P1485 S1486 K1487 V1492
R1493 V1496 Y1499 L1503 R1507 V1508 L1509 E1512 R1518 P1521 T1533 N1534 E1535 Y1538 Y1539 L1540 D1541 I1542 Y1545 T1549 ASP SER ARG THR A1554 Q1555 I1556 M1557 F1558 Q1559 A1560 TYR GLY ASP K1564 Q1565 G1566 P1567 L1568 M1571 L1572 I1573 V1578 T1579 K1580 L1583

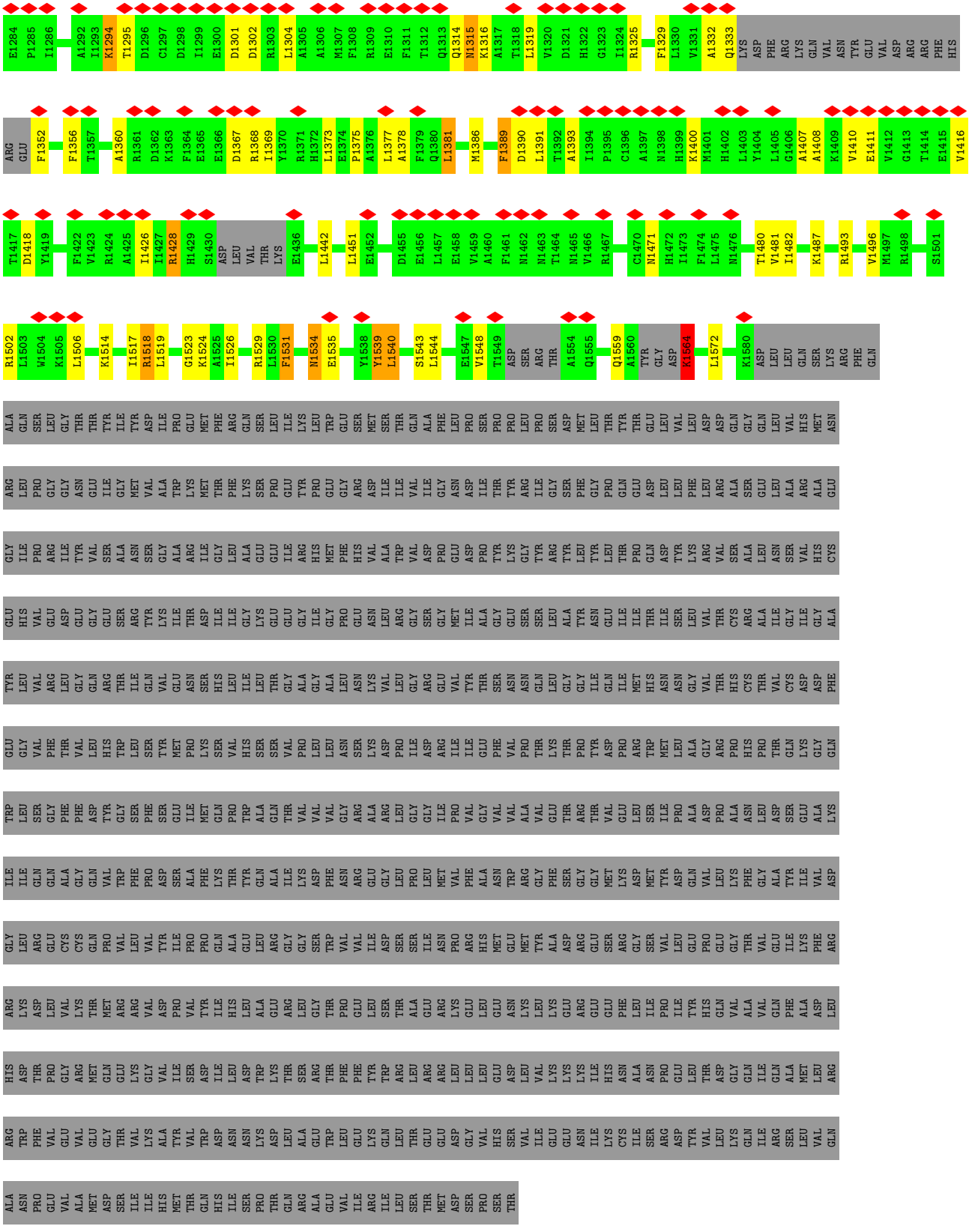


• Molecule 1: Acetyl-CoA carboxylase 1

Chain B:

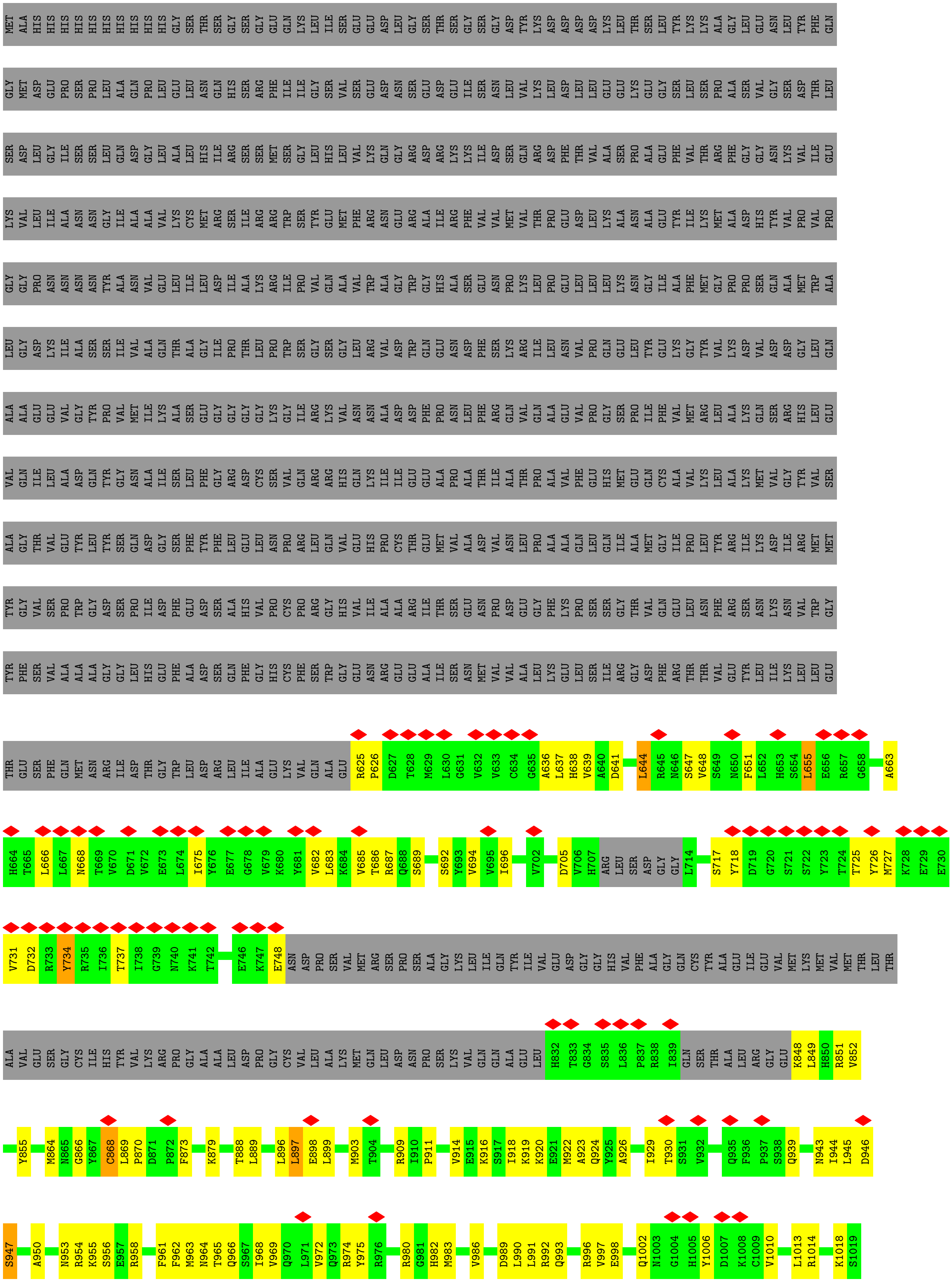






- Molecule 1: Acetyl-CoA carboxylase 1

Chain A: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GLY MET ASP GLU PRO SER PRO LEU ALA GLN PRO LEU GLU LEU ASN GLN HIS SER ARG PHE ILE ILE GLY SER VAL SER GLU ASP ASN SER GLU ASP GLU ILE SER ASN LEU VAL LYS LEU ASP LEU LEU GLU GLU LYS GLU GLY SER LEU SER PRO ALA SER VAL GLY SER ASP THR LEU
SER ASP LEU GLY ILE SER SER LEU GLN ASP GLY LEU ALA LEU HIS ILE ARG SER SER MET SER GLY LEU HIS LEU VAL LYS GLN GLY ARG ASP ARG LYS LYS ILE ASP SER GLN ARG ASP PHE THR VAL ALA SER PRO ALA GLU PHE VAL THR ARG PHE GLY GLY ASN LYS VAL ILE GLU
LYS VAL LEU ILE ALA ASN ASN GLY ILE ALA ALA VAL LYS CYS MET ARG SER ILE ARG ARG TRP SER TYR GLU MET PHE ARG ASN GLU ARG ALA ILE ARG PHE VAL VAL MET VAL THR PRO GLU ASP LEU LYS ALA ASN ALA GLU TYR ILE LYS MET ALA ASP HIS TYR VAL PRO VAL PRO
GLY GLY PRO ASN ASN ASN TYR ALA ASN VAL GLU LEU ILE LEU ASP ILE ALA LYS ARG ILE PRO VAL GLN ALA VAL TRP ALA GLY TRP GLY HIS ALA SER GLU ASN PRO LYS LEU PRO GLU LEU LEU LEU LYS ASN GLY ILE ALA PHE MET GLY PRO PRO SER GLN ALA MET TRP ALA
LEU GLY ASP LYS ILE ALA SER SER ILE VAL ALA GLN THR ALA GLY ILE PRO THR LEU PRO TRP SER GLY SER GLY LEU ARG VAL ASP TRP GLN GLU ASN ASP PHE SER LYS ARG ILE LEU ASN VAL PRO GLN GLU LEU TYR GLU LYS GLY TYR VAL LYS ASP VAL ASP ASP GLY LEU GLN
ALA ALA GLU GLU VAL GLY TYR PRO VAL MET ILE LYS ALA SER GLU GLY GLY GLY GLY LYS GLY ILE ARG LYS VAL ASN ASN ALA ASP ASP PHE PRO ASN LEU PHE ARG GLN VAL GLN ALA GLU VAL PRO GLY SER PRO ILE PHE VAL MET ARG LEU ALA LYS GLN SER ARG HIS LEU GLU
VAL GLN ILE LEU ALA ASP GLN TYR GLY ASN ALA ILE SER LEU PHE GLY ARG ASP CYS SER VAL GLN ARG ARG HIS GLN LYS ILE ILE GLU GLU ALA PRO ALA THR ILE ALA THR PRO ALA VAL PHE GLU HIS MET GLU GLN CYS ALA VAL LYS LEU ALA LYS MET VAL GLY TYR VAL SER
ALA GLY THR VAL GLU TYR LEU TYR SER GLN ASP GLY SER PHE TYR PHE LEU GLU LEU ASN PRO ARG LEU GLN VAL GLU HIS PRO CYS THR GLU MET VAL ALA ASP VAL ASN LEU PRO ALA ALA GLN LEU GLN ILE ALA MET GLY ILE PRO LEU TYR ARG ILE LYS ASP ILE ARG MET MET
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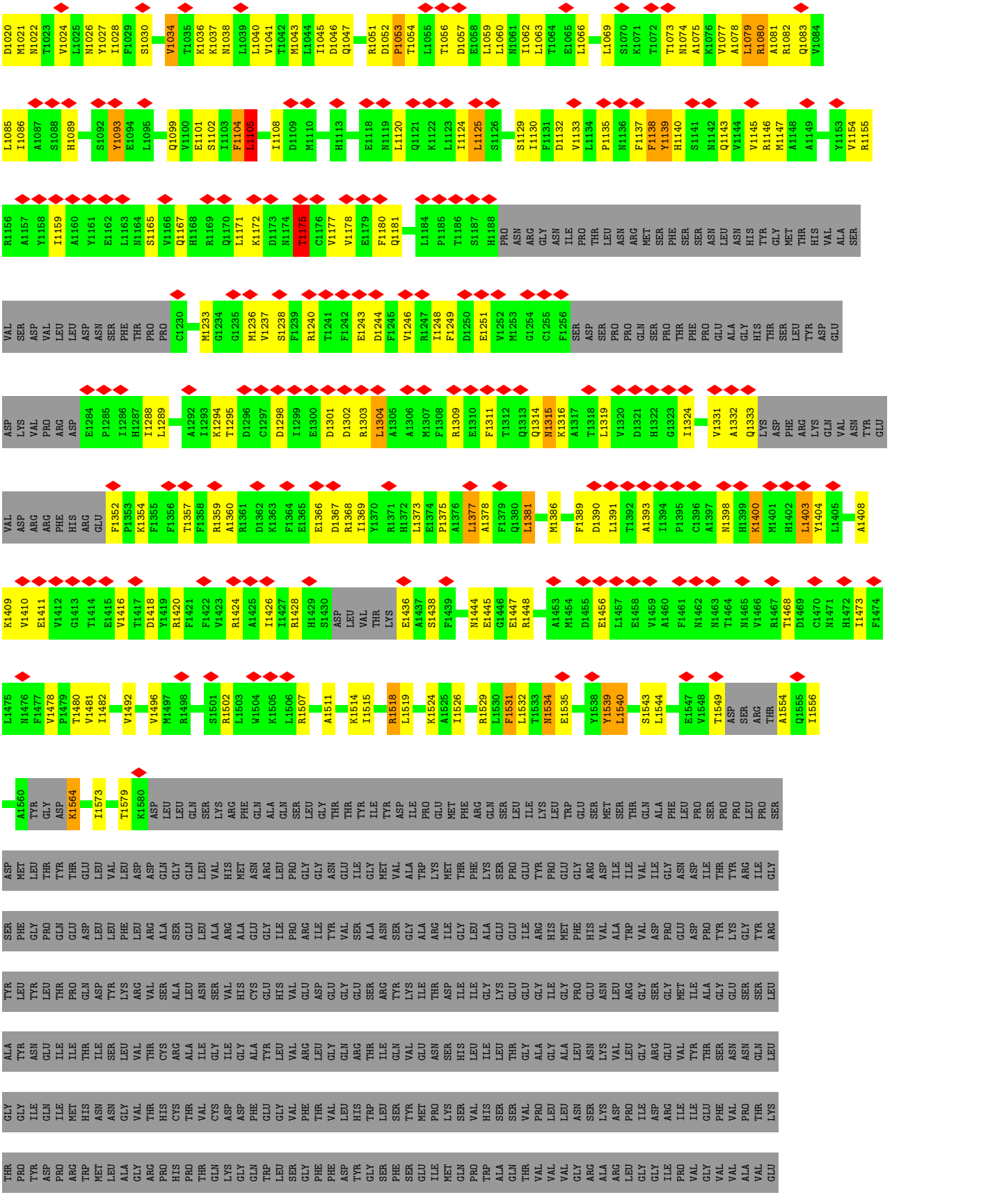
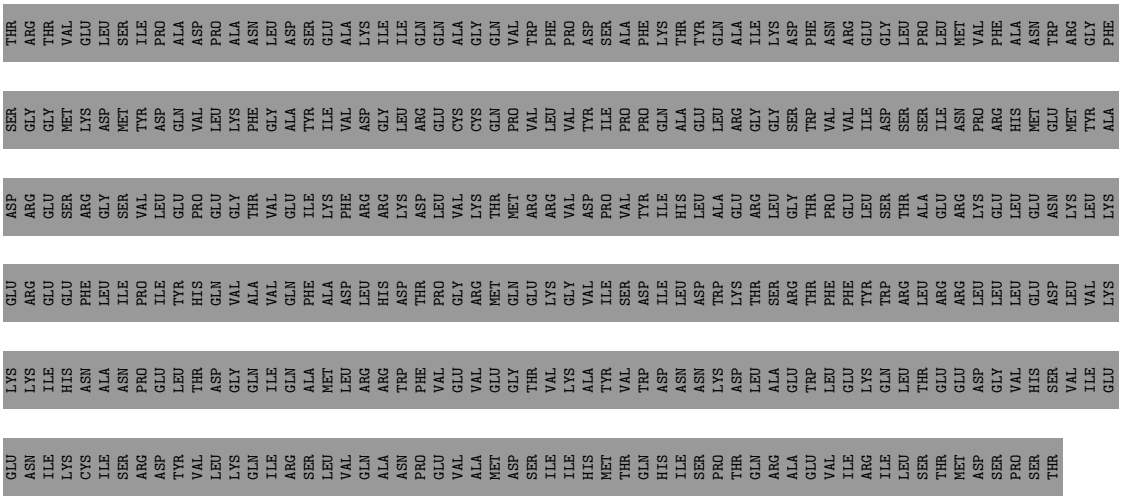
TYR PHE SER VAL ALA ALA ALA GLY GLY LEU HIS GLU PHE ALA ASP SER GLN PHE GLY HIS CYS PHE SER TRP GLY GLU ASN ARG GLU GLU ALA ILE SER ASN MET VAL VAL ALA LEU LYS GLU LEU SER ILE ARG GLY ASP PHE ARG THR THR VAL GLU TYR LEU ILE LYS LEU LEU GLU
THR GLU SER PHE GLN MET ASN ARG ILE ASP THR GLY TRP LEU ASP ARG LEU ILE ALA GLU LYS VAL GLN ALA GLU R625 P626 D627 T628 M629 L630 G631 V632 V633 C634 G635 A636 L637 H638 V639 A640 D641 L644 R645 N646 S647 V648 S649 N650 F651 L652 H653 S654 L655 E656 R657 G658 A663
H664 T665 L666 L667 N668 T669 V670 D671 V672 E673 L674 I675 Y676 E677 G678 V679 K680 Y681 V682 L683 K684 V685 T686 R687 Q688 S689 S692 Y693 V694 V695 I696 V702 D705 V706 H707 ARG LEU SER ASP GLY GLY L714 S717 Y718 D719 G720 S721 S722 Y723 T724 T725 Y726 M727 K728 E729 E730
V731 D732 R733 Y734 R735 I736 T737 I738 G739 N740 K741 T742 E746 K747 E748 ASN ASP PRO SER VAL MET ARG SER PRO SER ALA GLY LYS LEU ILE GLN TYR ILE VAL GLU ASP GLY GLY HIS VAL PHE ALA GLY GLN CYS TYR ALA GLU ILE GLU VAL MET LYS MET VAL MET THR LEU THR
ALA VAL GLU SER GLY CYS ILE HIS TYR VAL LYS ARG PRO GLY ALA ALA LEU ASP PRO GLY CYS VAL LEU ALA LYS MET GLN LEU ASP ASN PRO SER LYS VAL GLN GLN ALA GLU LEU H832 T833 G834 S835 L836 P837 R838 I839 GLN SER THR ALA LEU ARG GLY GLU K848 L849 H850 R851 V852
Y855 M864 N865 G866 Y867 C868 L869 P870 D871 P872 F873 K879 T888 L889 L896 L897 E898 L899 M903 T904 R909 I910 P911 V914 E915 K916 S917 I918 K919 K920 E921 M922 A923 Q924 Y925 A926 I929 T930 S931 V932 Q935 F936 P937 S938 Q939 N943 I944 L945 D946
S947 A950 N953 R954 K955 S956 E957 R958 F961 F962 M963 N964 T965 Q966 S967 I968 V969 Q970 L971 V972 Q973 R974 Y975 R976 R980 G981 H982 M983 V986 D989 L990 L991 R992 Q993 R996 V997 E998 Q1002 N1003 G1004 H1005 Y1006 D1007 K1008 C1009 V1010 L1013 R1014 K1018 S1019


D1020 M1021 N1022 T1023 V1024 L1025 N1026 Y1027 I1028 F1029 S1030 V1034 T1035 K1036 K1037 N1038 L1039 L1040 V1041 T1042 M1043 L1044 I1045 D1046 Q1047 R1051 D1052 P1053 T1054 L1055 T1056 D1057 E1058 L1059 L1060 N1061 I1062 L1063 T1064 E1065 L1066 L1069 S1070 K1071 T1072 T1073 N1074 A1075 K1076 V1077 A1078 L1079 R1080 A1081 R1082 Q1083 V1084
L1085 I1086 A1087 S1088 H1089 S1092 Y1093 E1094 L1095 Q1099 V1100 E1101 S1102 I1103 F1104 L1105 I1108 D1109 M1110 H1113 E1118 N1119 L1120 Q1121 K1122 L1123 I1124 L1125 S1126 S1129 I1130 F1131 D1132 V1133 L1134 P1135 N1136 F1137 F1138 Y1139 H1140 S1141 N1142 Q1143 V1144 V1145 R1146 M1147 A1148 A1149 Y1153 V1154 R1155
R1156 A1157 Y1158 I1159 A1160 Y1161 E1162 L1163 N1164 S1165 V1166 Q1167 H1168 R1169 Q1170 L1171 K1172 D1173 N1174 T1175 C1176 V1177 V1178 E1179 F1180 Q1181 L1184 P1185 T1186 S1187 H1188 PRO ASN ARG GLY ASN ILE PRO THR LEU ASN ARG MET SER PHE SER SER ASN LEU ASN HIS TYR GLY MET THR HIS VAL ALA SER
VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO C1230 M1233 G1234 G1235 M1236 V1237 S1238 F1239 R1240 T1241 F1242 E1243 D1244 F1245 V1246 R1247 I1248 F1249 D1250 E1251 V1252 M1253 G1254 C1255 F1256 SER ASP SER PRO PRO GLN SER PRO THR THR PHE PRO GLU ALA GLY HIS THR SER LEU TYR ASP GLU
ASP LYS VAL PRO ARG ASP E1284 P1285 I1286 H1287 I1288 L1289 A1292 I1293 K1294 T1295 D1296 C1297 D1298 I1299 E1300 D1301 D1302 R1303 L1304 A1305 A1306 M1307 F1308 R1309 E1310 F1311 T1312 Q1313 Q1314 N1315 K1316 A1317 T1318 L1319 V1320 D1321 H1322 G1323 I1324 V1331 A1332 Q1333 LYS ASP PHE ARG LYS GLN VAL ASN TYR GLU
VAL ASP ARG ARG PHE HIS ARG GLU F1352 P1353 K1354 F1355 F1356 T1357 F1358 R1359 A1360 R1361 D1362 K1363 F1364 E1365 E1366 D1367 R1368 I1369 Y1370 R1371 H1372 L1373 E1374 P1375 A1376 L1377 A1378 F1379 Q1380 L1381 M1386 F1389 D1390 L1391 T1392 A1393 I1394 P1395 C1396 A1397 N1398 H1399 K1400 M1401 H1402 L1403 Y1404 L1405 A1408
K1409 V1410 E1411 V1412 G1413 T1414 E1415 V1416 T1417 D1418 Y1419 R1420 F1421 F1422 V1423 R1424 A1425 I1426 T1427 R1428 H1429 S1430 ASP LEU VAL THR LYS E1436 A1437 S1438 F1439 N1444 E1445 G1446 E1447 R1448 A1453 M1454 D1455 E1456 L1457 E1458 V1459 A1460 F1461 N1462 N1463 T1464 N1465 V1466 R1467 T1468 D1469 C1470 N1471 H1472 I1473 F1474
L1475 N1476 F1477 V1478 P1479 T1480 V1481 I1482 V1492 V1496 M1497 R1498 S1501 R1502 L1503 W1504 K1505 L1506 R1507 A1511 K1514 I1515 R1518 L1519 K1524 A1525 I1526 R1529 L1530 F1531 L1532 T1533 N1534 E1535 Y1538 Y1539 L1540 S1543 L1544 E1547 V1548 T1549 ASP SER ARG THR A1554 Q1555 I1556
A1560 TYR GLY ASP K1564 I1573 T1579 K1580 ASP LEU LEU GLN SER LYS ARG PHE ASN GLN ALA GLN SER LEU GLY THR THR TYR ILE TYR ASP ILE PRO GLU MET PHE ARG GLN SER LEU ILE LYS LEU TRP GLU SER MET SER THR GLN ALA PHE LEU PRO SER PRO PRO LEU PRO SER
ASP MET LEU THR TYR THR GLU LEU VAL LEU ASP ASP GLN GLY GLN LEU VAL HIS MET ASN ARG LEU PRO GLY GLY ASN GLU ILE GLY MET VAL ALA TRP LYS MET THR PHE LYS SER PRO GLU TYR PRO GLU GLY ARG ASP ILE ILE VAL ALA ILE GLY ASN ASP ILE THR TYR ARG ILE GLY
SER PHE GLY PRO GLN GLU ASP LEU LEU PHE LEU ARG ALA SER GLU LEU ALA ARG ALA GLU GLY ILE PRO ARG ILE TYR VAL SER ALA ASN SER GLY ALA ARG ILE GLY PHE LEU ALA GLU GLU ILE ARG HIS MET PHE HIS VAL ALA TRP VAL ASP PRO GLU ASP PRO TYR LYS GLY TYR ARG
TYR LEU TYR LEU THR PRO GLN ASP TYR LYS ARG VAL SER ALA LEU ASN SER VAL HIS CYS GLU HIS VAL GLU ASP GLU GLY GLU SER ARG TYR LYS ILE THR ASP ILE ILE GLY LYS GLU GLU GLY ILE GLY PRO GLU ASN LEU ARG GLY SER GLY MET ILE ALA GLY GLU SER SER LEU
ALA TYR ASN GLU ILE ILE THR ILE SER LEU VAL ARG LEU GLY GLN ARG THR ILE GLN VAL GLU ASN SER HIS LEU ILE LEU LEU THR GLY ALA GLY ALA LEU ASN ASN LYS VAL LEU GLY ARG GLU VAL TYR THR SER ASN ASN GLN LEU
GLY GLY ILE GLN ILE MET HIS ASN ASN GLY VAL THR HIS CYS THR VAL CYS ASP ASP PHE GLU GLY VAL PHE THR VAL LEU HIS TRP LEU SER TYR MET THR SER VAL HIS SER SER VAL PRO LEU LEU ASN SER LYS ASP PRO ILE ASP ILE ILE GLU PHE VAL PRO THR LYS
THR PRO TYR ASP PRO ARG TRP MET LEU ALA GLY ARG PRO HIS PRO THR GLN LYS GLY GLN TRP LEU SER GLY PHE PHE ASP TYR GLY SER PHE SER GLU ILE MET GLN PRO TRP ALA GLN THR VAL VAL VAL GLY ARG ALA ARG LEU GLY GLY ILE PRO VAL GLY PHE VAL ALA GLY GLU VAL PRO ILE GLY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SER GLY GLY MET LYS ASP MET TYR ASP GLN VAL LEU LYS PHE GLY ALA TYR ILE VAL ASP GLY LEU ARG GLU CYS GLN PRO VAL LEU VAL TYR ILE PRO PRO GLN ALA GLU LEU ARG GLY GLY SER TRP VAL VAL ILE ASP SER SER ILE ASN PRO ARG HIS MET GLU MET TYR ALA
ASP ARG GLU SER ARG GLY SER VAL LEU GLU PRO GLU GLY THR VAL GLU ILE LYS PHE ARG ARG LYS ASP LEU VAL LYS THR MET ARG ARG VAL ASP PRO VAL TYR ILE HIS LEU ALA GLU ARG LEU GLY THR PRO GLU LEU SER THR ALA GLU ARG LYS GLU LEU GLU ASN LYS LEU LYS
GLU ARG GLU GLU PHE LEU ILE PRO ILE TYR HIS GLN VAL ALA VAL GLN PHE ALA ASP LEU HIS ASP THR PRO GLY ARG MET GLN GLU LYS GLY VAL ILE SER ASP ILE LEU ASP TRP LYS THR SER ARG THR PHE PHE TYR TRP ARG LEU ARG ARG LEU LEU LEU GLU ASP LEU VAL LYS
LYS LYS ILE HIS ASN ALA ASN PRO GLU LEU THR ASP GLY GLN ILE GLN ALA MET LEU ARG ARG TRP PHE VAL GLU VAL GLU GLY THR VAL LYS ALA TYR VAL TRP ASP ASN ASN LYS ASP LEU ALA GLU TRP LEU GLU LYS GLN LEU THR GLU GLU ASP GLY VAL HIS SER VAL ILE GLU
GLU ASN ILE LYS CYS ILE SER ARG ASP TYR VAL LEU LYS GLN ILE ARG SER LEU VAL GLN ALA ASN PRO GLU VAL ALA MET ASP SER ILE ILE HIS MET THR GLN HIS ILE SER PRO THR GLN ARG ALA GLU VAL ILE ARG ILE LEU SER THR MET ASP SER PRO SER THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	48483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	397.80798, 397.80798, 397.80798	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	0/6291	1.08	26/8496 (0.3%)
1	B	0.51	0/6291	1.05	24/8496 (0.3%)
1	C	0.64	3/7780 (0.0%)	0.99	13/10540 (0.1%)
1	D	0.65	1/12491 (0.0%)	1.07	53/16905 (0.3%)
1	E	0.64	1/12491 (0.0%)	1.05	48/16905 (0.3%)
1	F	0.64	1/7780 (0.0%)	1.01	24/10540 (0.2%)
All	All	0.62	6/53124 (0.0%)	1.04	188/71882 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	10
1	C	0	1
1	D	0	16
1	E	0	11
1	F	0	1
All	All	0	51

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2018	TRP	CB-CG	-6.72	1.38	1.50
1	D	1895	VAL	CB-CG1	-6.51	1.39	1.52
1	E	2046	TRP	CB-CG	-5.25	1.40	1.50
1	F	2018	TRP	CB-CG	-5.24	1.40	1.50
1	C	2046	TRP	CB-CG	-5.08	1.41	1.50
1	C	1738	TRP	CB-CG	-5.01	1.41	1.50

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1503	LEU	CA-CB-CG	11.38	141.47	115.30
1	A	1381	LEU	CA-CB-CG	10.26	138.91	115.30
1	F	1539	TYR	CB-CG-CD2	-10.03	114.98	121.00
1	F	1691	PHE	CB-CG-CD2	-9.57	114.10	120.80
1	E	651	PHE	CB-CG-CD2	-9.28	114.30	120.80
1	B	1531	PHE	CB-CG-CD1	-9.23	114.34	120.80
1	C	1507	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	B	1381	LEU	CA-CB-CG	8.88	135.72	115.30
1	B	1531	PHE	CB-CG-CD2	8.82	126.98	120.80
1	D	1449	LEU	CB-CG-CD1	8.65	125.70	111.00
1	E	2061	LEU	CA-CB-CG	8.37	134.56	115.30
1	D	1249	PHE	CB-CG-CD2	-8.34	114.96	120.80
1	A	909	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	E	1449	LEU	CB-CG-CD1	8.26	125.03	111.00
1	A	909	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	D	1079	LEU	CA-CB-CG	-8.02	96.86	115.30
1	C	1687	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	F	1691	PHE	CB-CG-CD1	7.72	126.21	120.80
1	E	651	PHE	CB-CG-CD1	7.71	126.20	120.80
1	E	2127	LYS	CD-CE-NZ	7.64	129.27	111.70
1	D	1249	PHE	CB-CG-CD1	7.58	126.11	120.80
1	F	1441	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	E	1381	LEU	CA-CB-CG	7.47	132.49	115.30
1	F	1539	TYR	CB-CG-CD1	7.46	125.47	121.00
1	E	1125	LEU	CA-CB-CG	7.44	132.40	115.30
1	F	1441	TYR	CB-CG-CD1	7.36	125.42	121.00
1	B	1442	LEU	CA-CB-CG	7.22	131.91	115.30
1	B	909	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	1539	TYR	CB-CG-CD1	7.18	125.31	121.00
1	D	1545	TYR	C-N-CA	7.16	139.60	121.70
1	D	1389	PHE	CB-CG-CD2	-7.15	115.79	120.80
1	D	1085	LEU	CA-CB-CG	7.15	131.74	115.30
1	A	1539	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	A	644	LEU	CA-CB-CG	6.99	131.38	115.30
1	E	644	LEU	CB-CG-CD1	6.95	122.82	111.00
1	E	1403	LEU	CA-CB-CG	6.90	131.17	115.30
1	E	1359	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	D	1426	ILE	CG1-CB-CG2	6.87	126.52	111.40
1	D	1978	LEU	CB-CG-CD2	6.87	122.67	111.00
1	F	1441	TYR	CA-CB-CG	6.86	126.43	113.40
1	D	2133	LEU	CA-CB-CG	6.81	130.96	115.30
1	F	2189	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	909	ARG	NE-CZ-NH2	-6.78	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1441	TYR	CA-CB-CG	6.77	126.26	113.40
1	D	2038	LEU	CA-CB-CG	6.74	130.81	115.30
1	D	2035	ARG	CG-CD-NE	-6.67	97.79	111.80
1	C	2189	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	655	LEU	CA-CB-CG	6.62	130.53	115.30
1	F	1509	LEU	CB-CG-CD1	6.62	122.25	111.00
1	D	1077	VAL	CG1-CB-CG2	6.62	121.49	110.90
1	C	1991	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	1104	PHE	CB-CG-CD2	-6.55	116.21	120.80
1	F	1640	ASP	CB-CG-OD1	6.55	124.19	118.30
1	E	683	LEU	CA-CB-CG	6.51	130.27	115.30
1	D	1373	LEU	CB-CG-CD1	6.48	122.01	111.00
1	D	1359	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	D	1488	ILE	CG1-CB-CG2	6.48	125.65	111.40
1	C	1640	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	1377	LEU	CA-CB-CG	6.39	130.00	115.30
1	D	1473	ILE	CG1-CB-CG2	6.37	125.41	111.40
1	E	2133	LEU	CA-CB-CG	6.32	129.85	115.30
1	E	1249	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	F	1401	MET	CG-SD-CE	6.29	110.27	100.20
1	B	868	CYS	CA-CB-SG	6.29	125.32	114.00
1	A	1531	PHE	CB-CG-CD1	-6.27	116.41	120.80
1	D	1478	VAL	CG1-CB-CG2	6.25	120.89	110.90
1	E	1645	LEU	CB-CG-CD1	6.24	121.61	111.00
1	D	1531	PHE	CB-CG-CD2	6.19	125.13	120.80
1	E	2221	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	E	2111	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	1156	ARG	CG-CD-NE	6.12	124.64	111.80
1	E	1156	ARG	CG-CD-NE	6.10	124.61	111.80
1	F	1731	ARG	CB-CA-C	-6.09	98.22	110.40
1	A	1514	LYS	CD-CE-NZ	6.08	125.69	111.70
1	A	1403	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	1498	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	1308	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	D	1978	LEU	CB-CG-CD1	-6.00	100.79	111.00
1	F	1687	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	1428	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	E	2336	ARG	CB-CG-CD	5.94	127.04	111.60
1	D	1531	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	E	889	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	2221	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	1104	PHE	CB-CG-CD2	-5.87	116.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1485	PRO	N-CA-C	5.85	127.30	112.10
1	A	644	LEU	CB-CG-CD2	5.84	120.93	111.00
1	D	1837	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	E	2221	ARG	CG-CD-NE	-5.83	99.56	111.80
1	C	1937	MET	CA-CB-CG	5.83	123.21	113.30
1	B	1066	LEU	CA-CB-CG	5.82	128.69	115.30
1	D	1662	TRP	CB-CA-C	-5.81	98.77	110.40
1	A	1105	LEU	CB-CG-CD2	5.81	120.88	111.00
1	D	1403	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	1105	LEU	CB-CG-CD2	5.79	120.85	111.00
1	A	1377	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	D	1459	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	D	2035	ARG	CB-CG-CD	5.76	126.58	111.60
1	F	2139	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	2128	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	E	990	LEU	CA-CB-CG	5.71	128.43	115.30
1	E	1428	ARG	CB-CA-C	5.71	121.81	110.40
1	F	2068	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	F	2118	LEU	CB-CG-CD1	5.70	120.69	111.00
1	D	1367	ASP	CB-CG-OD1	5.70	123.43	118.30
1	F	1938	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	2220	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	E	2111	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	E	1249	PHE	CB-CG-CD1	5.66	124.76	120.80
1	D	1428	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	1294	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	D	718	TYR	CB-CA-C	5.64	121.68	110.40
1	D	1079	LEU	CB-CG-CD2	5.62	120.56	111.00
1	E	1854	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	1093	TYR	CB-CA-C	5.59	121.58	110.40
1	D	2220	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	1080	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	1531	PHE	CB-CG-CD2	5.57	124.70	120.80
1	B	1367	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	1085	LEU	CA-CB-CG	5.55	128.07	115.30
1	E	718	TYR	CB-CA-C	5.54	121.47	110.40
1	A	718	TYR	CB-CA-C	5.52	121.44	110.40
1	D	1662	TRP	CA-CB-CG	5.52	124.19	113.70
1	D	1079	LEU	CB-CG-CD1	5.47	120.30	111.00
1	E	1723	ARG	CG-CD-NE	5.47	123.28	111.80
1	E	1640	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	1093	TYR	CB-CA-C	5.46	121.33	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1758	TYR	CA-CB-CG	5.46	123.77	113.40
1	F	1833	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	1125	LEU	CA-CB-CG	5.42	127.78	115.30
1	E	2227	LEU	CA-CB-CG	5.41	127.75	115.30
1	E	2079	LEU	CA-CB-CG	5.41	127.74	115.30
1	E	1428	ARG	N-CA-C	-5.40	96.41	111.00
1	D	1105	LEU	CB-CG-CD2	5.40	120.19	111.00
1	B	718	TYR	CB-CA-C	5.40	121.19	110.40
1	A	980	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	1021	MET	CA-CB-CG	5.39	122.46	113.30
1	F	1937	MET	CA-CB-CG	5.37	122.43	113.30
1	D	1428	ARG	CA-CB-CG	5.36	125.20	113.40
1	E	1180	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	E	1327	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	1053	PRO	N-CA-C	5.35	126.00	112.10
1	E	1731	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	E	2221	ARG	CB-CA-C	-5.33	99.75	110.40
1	B	884	ARG	CA-CB-CG	5.33	125.11	113.40
1	C	1938	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	2179	TYR	CB-CG-CD1	5.31	124.19	121.00
1	F	1381	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	1079	LEU	CA-CB-CG	5.29	127.46	115.30
1	E	1687	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	1622	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	2179	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	651	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	F	2220	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	1055	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	1797	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	868	CYS	CA-CB-SG	5.24	123.42	114.00
1	B	1529	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	1389	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	B	1493	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1139	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	2118	LEU	CB-CG-CD1	5.19	119.82	111.00
1	E	1609	LEU	CA-CB-CG	5.18	127.21	115.30
1	D	2168	LEU	CA-CB-CG	5.18	127.20	115.30
1	A	1529	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	1422	PHE	N-CA-CB	5.16	119.89	110.60
1	E	1975	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	1424	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	990	LEU	CB-CG-CD1	5.11	119.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1662	TRP	CB-CA-C	-5.11	100.17	110.40
1	D	1450	LEU	CA-CB-CG	5.11	127.06	115.30
1	D	1723	ARG	CG-CD-NE	5.10	122.51	111.80
1	F	1662	TRP	CA-CB-CG	5.10	123.39	113.70
1	F	2336	ARG	CG-CD-NE	5.10	122.51	111.80
1	D	1632	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	E	2168	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	1539	TYR	CB-CG-CD1	5.09	124.05	121.00
1	D	2250	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	971	LEU	CA-CB-CG	5.08	126.99	115.30
1	F	2179	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	1125	LEU	CA-CB-CG	5.08	126.97	115.30
1	C	2038	LEU	CA-CB-CG	5.07	126.96	115.30
1	E	1389	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	B	1104	PHE	CB-CG-CD1	5.05	124.33	120.80
1	C	1441	TYR	CA-CB-CG	5.05	122.99	113.40
1	B	909	ARG	CD-NE-CZ	5.05	130.66	123.60
1	C	2107	MET	CA-CB-CG	5.02	121.83	113.30
1	A	1359	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	ARG	Peptide
1	A	1052	ASP	Peptide
1	A	1054	THR	Peptide
1	A	1171	LEU	Peptide
1	A	1175	THR	Peptide
1	A	1249	PHE	Peptide
1	A	1294	LYS	Peptide
1	A	1295	THR	Peptide
1	A	1315	ASN	Peptide
1	A	1332	ALA	Peptide
1	A	1564	LYS	Peptide
1	A	924	GLN	Peptide
1	B	1052	ASP	Peptide
1	B	1171	LEU	Peptide
1	B	1249	PHE	Peptide
1	B	1315	ASN	Peptide
1	B	1332	ALA	Peptide
1	B	1564	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	924	GLN	Peptide
1	B	957	GLU	Peptide
1	B	963	MET	Mainchain
1	B	965	THR	Mainchain
1	C	1564	LYS	Peptide
1	D	1052	ASP	Peptide
1	D	1087	ALA	Peptide
1	D	1110	MET	Peptide
1	D	1118	GLU	Sidechain
1	D	1171	LEU	Peptide
1	D	1175	THR	Peptide
1	D	1249	PHE	Peptide
1	D	1298	ASP	Peptide
1	D	1315	ASN	Peptide
1	D	1332	ALA	Peptide
1	D	1425	ALA	Peptide
1	D	1564	LYS	Peptide
1	D	924	GLN	Peptide
1	D	952	LEU	Peptide
1	D	957	GLU	Peptide
1	D	965	THR	Mainchain
1	E	1052	ASP	Peptide
1	E	1110	MET	Peptide
1	E	1171	LEU	Peptide
1	E	1249	PHE	Peptide
1	E	1298	ASP	Peptide
1	E	1315	ASN	Peptide
1	E	1332	ALA	Peptide
1	E	1547	GLU	Peptide
1	E	1564	LYS	Peptide
1	E	924	GLN	Peptide
1	E	957	GLU	Peptide
1	F	1564	LYS	Peptide

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	6177	6184	6209	190	0
1	B	6177	6184	6209	175	0
1	C	7610	7561	7585	204	0
1	D	12235	12181	12225	363	0
1	E	12235	12181	12225	351	0
1	F	7610	7561	7585	204	0
All	All	52044	51852	52038	1406	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 14.

All (1406) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1679:VAL:HG22	1:D:1714:ILE:HD11	1.54	0.88
1:C:2067:ILE:HD11	1:C:2095:VAL:HG12	1.54	0.88
1:E:668:ASN:ND2	1:E:868:CYS:SG	2.47	0.87
1:F:1545:TYR:OH	1:F:1567:PRO:O	1.92	0.87
1:E:2139:ARG:NH1	1:F:1734:PHE:O	2.08	0.87
1:C:1545:TYR:OH	1:C:1567:PRO:O	1.92	0.87
1:A:1480:THR:OG1	1:A:1518:ARG:NH1	2.08	0.86
1:C:2323:THR:O	1:C:2327:SER:OG	1.94	0.86
1:D:1545:TYR:OH	1:D:1567:PRO:O	1.94	0.86
1:E:2095:VAL:HG23	1:E:2096:ILE:HG23	1.59	0.85
1:F:1612:LEU:HD22	1:F:1896:LEU:HD13	1.59	0.84
1:D:972:VAL:O	1:D:976:ARG:N	2.10	0.84
1:D:1539:TYR:CE1	1:D:1629:SER:HA	2.12	0.84
1:F:2323:THR:O	1:F:2327:SER:OG	1.94	0.84
1:D:1803:ILE:HD13	1:D:1831:LEU:HD11	1.59	0.83
1:E:972:VAL:O	1:E:976:ARG:N	2.11	0.83
1:D:2240:THR:OG1	1:D:2243:GLN:OE1	1.96	0.83
1:B:1014:ARG:O	1:B:1018:LYS:HA	1.79	0.83
1:A:1014:ARG:O	1:A:1018:LYS:HA	1.78	0.83
1:E:1063:LEU:HD12	1:E:1085:LEU:HD13	1.62	0.82
1:D:2139:ARG:NH1	1:C:1734:PHE:O	2.13	0.82
1:A:1534:ASN:ND2	1:A:1539:TYR:O	2.13	0.81
1:B:1534:ASN:ND2	1:B:1539:TYR:O	2.13	0.81
1:C:1480:THR:OG1	1:C:1518:ARG:NH1	2.14	0.81
1:F:1923:ILE:O	1:F:2209:LYS:NZ	2.13	0.81
1:C:1655:ASN:ND2	1:C:1659:MET:O	2.14	0.80
1:F:1655:ASN:ND2	1:F:1659:MET:O	2.15	0.80
1:D:1784:ASP:OD1	1:C:2192:THR:OG1	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2095:VAL:HG23	1:D:2096:ILE:HG23	1.63	0.80
1:D:1975:ARG:NH2	1:D:2032:ASP:OD2	2.15	0.79
1:E:1716:VAL:HG22	1:E:1819:LEU:HD21	1.63	0.79
1:E:1385:ARG:NH2	1:E:1512:GLU:OE2	2.15	0.79
1:F:1727:ALA:HB3	1:F:1785:ILE:HD11	1.65	0.79
1:A:1140:HIS:O	1:A:1146:ARG:NH2	2.14	0.79
1:A:1069:LEU:HD11	1:A:1078:ALA:HB2	1.63	0.79
1:F:1811:TYR:OH	1:F:2032:ASP:OD1	2.01	0.79
1:D:1764:LEU:O	1:D:1788:LYS:NZ	2.16	0.78
1:E:2066:TYR:OH	1:F:2028:GLN:OE1	2.01	0.78
1:F:1480:THR:OG1	1:F:1518:ARG:NH1	2.17	0.78
1:B:1531:PHE:O	1:B:1543:SER:OG	2.01	0.78
1:E:1545:TYR:OH	1:E:1567:PRO:O	2.00	0.78
1:A:1531:PHE:O	1:A:1543:SER:OG	2.00	0.78
1:F:1385:ARG:NH1	1:F:1512:GLU:OE2	2.16	0.77
1:D:1745:TYR:OH	1:C:2174:PHE:O	2.02	0.77
1:B:1368:ARG:HG3	1:B:1393:ALA:HB3	1.66	0.77
1:D:1716:VAL:HG22	1:D:1819:LEU:HD21	1.64	0.77
1:C:2016:GLN:HE21	1:C:2045:ASN:HD21	1.30	0.77
1:D:1682:ASN:ND2	1:D:1718:ALA:O	2.18	0.77
1:E:1146:ARG:NH1	1:E:1238:SER:O	2.18	0.77
1:F:2156:LEU:O	1:F:2161:ARG:NH1	2.18	0.77
1:A:1132:ASP:OD1	1:A:1333:GLN:NE2	2.17	0.77
1:B:898:GLU:OE1	1:B:975:TYR:OH	2.03	0.77
1:C:2156:LEU:O	1:C:2161:ARG:NH1	2.18	0.76
1:A:1143:GLN:NE2	1:A:1147:MET:SD	2.59	0.76
1:A:1137:PHE:O	1:A:1140:HIS:ND1	2.15	0.76
1:D:979:ILE:HD12	1:D:980:ARG:HD3	1.67	0.76
1:C:2291:ASN:O	1:C:2295:ILE:HD12	1.86	0.76
1:E:972:VAL:HG22	1:E:976:ARG:HB3	1.67	0.76
1:D:1954:PHE:O	1:D:2212:ARG:NH1	2.18	0.75
1:E:1471:ASN:ND2	1:E:1506:LEU:O	2.19	0.75
1:E:1910:VAL:HG23	1:E:1912:LEU:HD21	1.69	0.75
1:E:1923:ILE:HD11	1:E:2212:ARG:HB2	1.69	0.75
1:D:1114:GLN:HE21	1:D:1148:ALA:HB2	1.52	0.75
1:D:1386:MET:SD	1:D:1424:ARG:NH2	2.60	0.75
1:E:1954:PHE:O	1:E:2212:ARG:NH1	2.19	0.75
1:C:1700:LEU:HB2	1:C:1803:ILE:HD11	1.68	0.75
1:B:1132:ASP:OD1	1:B:1333:GLN:NE2	2.19	0.75
1:D:2195:ARG:NE	1:C:1786:ILE:O	2.19	0.74
1:C:2319:ILE:O	1:C:2323:THR:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:ILE:O	1:A:1089:HIS:N	2.19	0.74
1:F:2315:ALA:O	1:F:2318:SER:OG	2.02	0.74
1:E:2050:SER:OG	1:E:2055:ASP:OD2	2.05	0.74
1:D:951:THR:O	1:D:954:ARG:NH1	2.21	0.74
1:E:1470:CYS:HA	1:E:1509:LEU:HD21	1.70	0.74
1:B:1046:ASP:OD1	1:B:1080:ARG:NH1	2.20	0.74
1:F:2325:HIS:O	1:F:2327:SER:OG	2.06	0.73
1:B:705:ASP:O	1:B:717:SER:OG	2.05	0.73
1:F:2089:ARG:NH1	1:F:2116:SER:OG	2.21	0.73
1:D:2050:SER:OG	1:D:2055:ASP:OD2	2.05	0.73
1:F:2319:ILE:O	1:F:2323:THR:HG23	1.89	0.73
1:D:1086:ILE:O	1:D:1089:HIS:N	2.21	0.73
1:E:706:VAL:HG23	1:E:716:LEU:HD12	1.69	0.73
1:D:1471:ASN:ND2	1:D:1507:ARG:O	2.21	0.73
1:A:1544:LEU:O	1:A:1564:LYS:NZ	2.20	0.73
1:D:2089:ARG:NH1	1:D:2116:SER:OG	2.22	0.72
1:E:1245:PHE:O	1:E:1248:ILE:N	2.22	0.72
1:A:1480:THR:O	1:A:1518:ARG:NH1	2.22	0.72
1:D:1472:HIS:ND1	1:D:1510:GLN:OE1	2.22	0.72
1:C:1670:GLU:OE2	1:C:1675:ARG:NH1	2.23	0.72
1:E:1114:GLN:HE21	1:E:1148:ALA:HB2	1.54	0.72
1:C:2325:HIS:O	1:C:2327:SER:OG	2.07	0.72
1:E:951:THR:O	1:E:954:ARG:NH1	2.22	0.72
1:A:989:ASP:OD1	1:A:990:LEU:N	2.23	0.72
1:D:1007:ASP:O	1:D:1010:VAL:HG12	1.90	0.71
1:E:961:PHE:O	1:E:965:THR:HG22	1.90	0.71
1:E:1745:TYR:OH	1:F:2174:PHE:O	2.08	0.71
1:C:2089:ARG:NH1	1:C:2116:SER:OG	2.23	0.71
1:D:2221:ARG:HD2	1:D:2271:ALA:HB2	1.73	0.71
1:A:1375:PRO:HA	1:A:1378:ALA:HB3	1.72	0.71
1:F:2291:ASN:O	1:F:2295:ILE:HD12	1.91	0.71
1:C:1463:ASN:OD1	1:C:1464:THR:N	2.23	0.71
1:C:1864:THR:OG1	1:C:1868:GLN:NE2	2.24	0.71
1:D:982:HIS:O	1:D:986:VAL:HG12	1.91	0.71
1:D:2044:ALA:O	1:D:2045:ASN:ND2	2.24	0.71
1:E:1102:SER:O	1:E:1106:SER:OG	2.06	0.70
1:C:1480:THR:O	1:C:1518:ARG:NH1	2.24	0.70
1:F:1864:THR:OG1	1:F:1868:GLN:NE2	2.24	0.70
1:B:886:MET:SD	1:B:890:ARG:NH2	2.64	0.70
1:D:1022:ASN:O	1:D:1026:ASN:ND2	2.25	0.70
1:F:1851:ALA:HB1	1:F:1863:TYR:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:PHE:O	1:D:965:THR:HG22	1.92	0.69
1:F:2246:ALA:HB3	1:A:946:ASP:OD1	1.92	0.69
1:D:1797:LEU:HD21	1:C:2093:TRP:CD1	2.28	0.69
1:A:926:ALA:O	1:A:929:ILE:HG22	1.92	0.69
1:A:1418:ASP:OD2	1:A:1579:THR:OG1	2.07	0.69
1:F:1670:GLU:OE2	1:F:1675:ARG:NH1	2.27	0.68
1:A:1368:ARG:HG3	1:A:1393:ALA:HB3	1.74	0.68
1:D:863:VAL:HG21	1:D:881:TRP:CZ3	2.28	0.68
1:D:940:GLN:O	1:D:944:ILE:HD12	1.92	0.68
1:C:1612:LEU:HD22	1:C:1896:LEU:HG	1.73	0.68
1:D:2021:ASP:OD1	1:D:2022:SER:N	2.26	0.68
1:F:2298:ASP:OD2	1:A:939:GLN:NE2	2.27	0.68
1:A:1038:ASN:ND2	1:A:1073:THR:O	2.26	0.68
1:D:1114:GLN:NE2	1:D:1144:VAL:O	2.27	0.68
1:E:2021:ASP:OD1	1:E:2022:SER:N	2.27	0.68
1:E:1238:SER:HA	1:E:1292:ALA:HB3	1.75	0.68
1:C:1851:ALA:HB1	1:C:1863:TYR:HB2	1.76	0.68
1:A:953:ASN:OD1	1:A:954:ARG:N	2.27	0.68
1:E:1007:ASP:O	1:E:1010:VAL:HG12	1.94	0.68
1:D:1499:TYR:CD2	1:D:1503:LEU:HD22	2.29	0.68
1:E:1837:ARG:NH1	1:E:2032:ASP:OD2	2.26	0.68
1:B:1132:ASP:O	1:B:1333:GLN:NE2	2.27	0.68
1:A:1132:ASP:O	1:A:1333:GLN:NE2	2.27	0.68
1:D:2132:ASP:OD1	1:C:1731:ARG:NH1	2.27	0.67
1:E:1472:HIS:HB2	1:E:1510:GLN:HE21	1.58	0.67
1:B:644:LEU:O	1:B:647:SER:OG	2.11	0.67
1:E:1375:PRO:HA	1:E:1378:ALA:HB3	1.76	0.67
1:F:1817:ILE:CD1	1:F:1899:LEU:HD21	2.25	0.67
1:B:953:ASN:OD1	1:B:954:ARG:N	2.28	0.67
1:A:644:LEU:O	1:A:647:SER:OG	2.12	0.67
1:D:1063:LEU:HD23	1:D:1085:LEU:HD23	1.77	0.67
1:E:966:GLN:HA	1:E:969:VAL:HG22	1.74	0.67
1:C:2246:ALA:HB3	1:B:946:ASP:OD1	1.94	0.67
1:A:638:HIS:ND1	1:A:727:MET:SD	2.68	0.67
1:E:1445:GLU:O	1:E:1449:LEU:HD13	1.95	0.67
1:C:1817:ILE:CD1	1:C:1899:LEU:HD21	2.24	0.67
1:A:1386:MET:SD	1:A:1424:ARG:NH2	2.68	0.67
1:D:1719:ASN:OD1	1:D:1720:SER:N	2.25	0.67
1:D:966:GLN:HA	1:D:969:VAL:HG22	1.76	0.67
1:D:1475:LEU:HD11	1:D:1477:PHE:CD1	2.30	0.67
1:B:1099:GLN:O	1:B:1102:SER:OG	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1924:GLU:O	1:E:2209:LYS:NZ	2.28	0.66
1:E:2296:SER:O	1:E:2300:VAL:HG23	1.95	0.66
1:F:1557:MET:SD	1:F:1559:GLN:NE2	2.68	0.66
1:F:1817:ILE:HD11	1:F:1899:LEU:HD21	1.77	0.66
1:E:1086:ILE:O	1:E:1089:HIS:N	2.28	0.66
1:B:889:LEU:HD21	1:B:982:HIS:HB2	1.76	0.66
1:D:2174:PHE:O	1:C:1745:TYR:OH	2.13	0.66
1:E:892:PRO:O	1:E:925:TYR:OH	2.09	0.66
1:E:2289:GLU:N	1:E:2289:GLU:OE1	2.28	0.66
1:B:892:PRO:HG2	1:B:929:ILE:HD11	1.78	0.66
1:A:923:ALA:O	1:A:926:ALA:HB3	1.96	0.66
1:E:1408:ALA:HB2	1:E:1418:ASP:HB3	1.77	0.66
1:D:2066:TYR:OH	1:C:2028:GLN:OE1	2.14	0.66
1:B:1022:ASN:O	1:B:1026:ASN:ND2	2.29	0.66
1:C:1557:MET:SD	1:C:1559:GLN:NE2	2.69	0.66
1:C:2201:VAL:HG23	1:C:2202:ILE:HG23	1.77	0.66
1:B:1178:VAL:HG12	1:B:1236:MET:HB3	1.76	0.66
1:D:1238:SER:HA	1:D:1292:ALA:HB3	1.77	0.65
1:B:997:VAL:HG22	1:B:1027:TYR:CE1	2.31	0.65
1:A:1099:GLN:O	1:A:1102:SER:OG	2.10	0.65
1:E:2089:ARG:NH1	1:E:2116:SER:OG	2.28	0.65
1:A:1082:ARG:NH2	1:A:1085:LEU:HD22	2.11	0.65
1:A:958:ARG:O	1:A:962:PHE:N	2.29	0.65
1:A:1022:ASN:O	1:A:1026:ASN:ND2	2.30	0.65
1:E:2132:ASP:OD1	1:F:1731:ARG:NH1	2.29	0.65
1:C:1811:TYR:OH	1:C:2032:ASP:OD1	2.15	0.65
1:A:1069:LEU:HD12	1:A:1069:LEU:O	1.95	0.65
1:D:1639:LEU:HD11	1:D:1643:GLY:HA2	1.79	0.65
1:E:863:VAL:HG21	1:E:881:TRP:CZ3	2.31	0.65
1:E:1020:ASP:OD1	1:E:1021:MET:N	2.30	0.65
1:A:961:PHE:O	1:A:965:THR:HG22	1.97	0.65
1:A:1132:ASP:OD1	1:A:1352:PHE:N	2.29	0.65
1:E:1682:ASN:ND2	1:E:1718:ALA:O	2.29	0.65
1:E:1900:SER:OG	1:E:1977:ARG:NH2	2.30	0.65
1:A:1357:THR:OG1	1:A:1367:ASP:OD1	2.04	0.65
1:F:1480:THR:O	1:F:1518:ARG:NH1	2.30	0.65
1:E:1114:GLN:NE2	1:E:1144:VAL:O	2.29	0.64
1:F:1696:ASP:O	1:F:1803:ILE:HD11	1.97	0.64
1:B:1082:ARG:NH2	1:B:1085:LEU:HD22	2.13	0.64
1:D:1359:ARG:NH1	1:D:1367:ASP:OD2	2.30	0.64
1:E:898:GLU:O	1:E:902:ILE:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:PRO:O	1:A:914:VAL:HG12	1.97	0.64
1:D:1020:ASP:OD1	1:D:1021:MET:N	2.31	0.64
1:B:1480:THR:O	1:B:1518:ARG:NH1	2.30	0.64
1:D:958:ARG:O	1:D:962:PHE:N	2.29	0.64
1:E:899:LEU:HD13	1:E:922:MET:SD	2.38	0.64
1:A:1178:VAL:HG12	1:A:1236:MET:HB3	1.80	0.64
1:E:1864:THR:OG1	1:E:1868:GLN:NE2	2.30	0.64
1:C:1843:ASN:ND2	1:C:1843:ASN:O	2.30	0.64
1:A:968:ILE:O	1:A:972:VAL:HG12	1.98	0.64
1:D:1076:LYS:HD3	1:D:1077:VAL:HG23	1.80	0.63
1:D:1968:ALA:HB3	1:D:2025:LYS:HD2	1.80	0.63
1:E:706:VAL:HG23	1:E:716:LEU:CD1	2.28	0.63
1:C:1817:ILE:HD11	1:C:1899:LEU:HD21	1.79	0.63
1:C:1671:TYR:OH	1:C:1904:LYS:N	2.30	0.63
1:B:1375:PRO:HA	1:B:1378:ALA:HB3	1.81	0.63
1:E:1822:CYS:SG	1:E:1823:ARG:N	2.72	0.63
1:F:1671:TYR:OH	1:F:1904:LYS:N	2.32	0.63
1:E:2291:ASN:O	1:E:2295:ILE:HD12	1.98	0.63
1:D:1595:THR:OG1	1:D:1596:THR:N	2.31	0.63
1:B:896:LEU:HD11	1:B:926:ALA:HB2	1.80	0.63
1:A:1172:LYS:NZ	1:A:1251:GLU:OE1	2.31	0.63
1:B:911:PRO:O	1:B:914:VAL:HG12	1.97	0.63
1:E:1595:THR:OG1	1:E:1596:THR:N	2.31	0.63
1:D:1372:HIS:O	1:D:1373:LEU:HG	1.99	0.62
1:D:1986:VAL:HG21	1:D:2030:ILE:HD11	1.81	0.62
1:F:1684:ILE:O	1:F:1688:ILE:HA	1.99	0.62
1:F:2243:GLN:NE2	1:A:947:SER:OG	2.32	0.62
1:C:1684:ILE:O	1:C:1688:ILE:HA	2.00	0.62
1:F:2123:THR:HG21	1:F:2187:ALA:HB1	1.81	0.62
1:B:1069:LEU:HD11	1:B:1078:ALA:HB2	1.82	0.62
1:D:1408:ALA:HB2	1:D:1418:ASP:HB3	1.80	0.62
1:D:2321:HIS:CE1	1:B:933:LEU:HD13	2.34	0.62
1:C:1471:ASN:ND2	1:C:1507:ARG:O	2.33	0.62
1:D:1769:CYS:SG	1:D:1770:GLU:N	2.73	0.62
1:B:889:LEU:HD22	1:B:983:MET:SD	2.39	0.62
1:D:995:LEU:HD22	1:D:1066:LEU:CD2	2.29	0.62
1:D:1896:LEU:HD23	1:D:1899:LEU:HD12	1.81	0.62
1:E:1971:VAL:HG13	1:E:2025:LYS:NZ	2.14	0.62
1:D:2196:MET:O	1:D:2201:VAL:HG22	1.99	0.62
1:C:2085:GLN:N	1:C:2112:GLU:O	2.32	0.62
1:E:958:ARG:O	1:E:962:PHE:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2336:ARG:HG3	1:E:2337:ILE:HD12	1.81	0.62
1:F:2221:ARG:NH2	1:F:2264:TRP:O	2.33	0.62
1:D:1797:LEU:HD11	1:C:2093:TRP:CD1	2.35	0.61
1:D:1864:THR:OG1	1:D:1868:GLN:NE2	2.33	0.61
1:E:1493:ARG:NH2	1:E:1542:ILE:HD11	2.15	0.61
1:C:1534:ASN:ND2	1:C:1539:TYR:O	2.33	0.61
1:A:896:LEU:HD11	1:A:926:ALA:HB2	1.82	0.61
1:D:660:VAL:HB	1:D:1010:VAL:HG11	1.83	0.61
1:A:1056:THR:OG1	1:A:1057:ASP:N	2.32	0.61
1:D:2124:VAL:O	1:D:2128:PHE:N	2.32	0.61
1:D:1038:ASN:OD1	1:D:1077:VAL:HG21	2.00	0.61
1:E:926:ALA:O	1:E:929:ILE:HG22	2.01	0.61
1:E:1695:GLU:O	1:E:1698:LEU:HD23	2.01	0.61
1:B:1481:VAL:HG22	1:B:1517:ILE:HG22	1.82	0.61
1:A:705:ASP:O	1:A:717:SER:OG	2.17	0.61
1:D:2089:ARG:NH2	1:D:2188:ASP:OD1	2.32	0.61
1:E:1925:PHE:O	1:E:2208:TRP:NE1	2.30	0.61
1:E:1718:ALA:HB1	1:E:1822:CYS:SG	2.41	0.61
1:A:866:GLY:HA3	1:A:1030:SER:HB2	1.83	0.61
1:E:990:LEU:HD12	1:E:991:LEU:N	2.16	0.61
1:E:1115:PHE:CE1	1:E:1117:ILE:HD13	2.35	0.61
1:B:1100:VAL:HA	1:B:1103:ILE:HG22	1.82	0.61
1:E:1167:GLN:N	1:E:1167:GLN:OE1	2.34	0.61
1:E:2124:VAL:O	1:E:2128:PHE:N	2.33	0.61
1:D:926:ALA:O	1:D:929:ILE:HG22	2.00	0.61
1:F:1622:LEU:HD12	1:F:1623:PRO:HD2	1.80	0.61
1:A:1177:VAL:HG22	1:A:1237:VAL:HG22	1.83	0.61
1:D:1531:PHE:O	1:D:1543:SER:OG	2.19	0.60
1:E:1480:THR:O	1:E:1480:THR:OG1	2.19	0.60
1:E:1547:GLU:O	1:E:1557:MET:O	2.19	0.60
1:E:2061:LEU:HD13	1:F:1848:LEU:HD11	1.81	0.60
1:B:968:ILE:O	1:B:972:VAL:HG12	2.01	0.60
1:D:1718:ALA:HB2	1:D:1821:THR:CG2	2.30	0.60
1:E:2331:ARG:O	1:E:2334:VAL:HG12	1.99	0.60
1:F:1680:ILE:HG21	1:F:1699:PHE:HD1	1.65	0.60
1:D:969:VAL:HG11	1:E:2250:ARG:HD2	1.83	0.60
1:E:1873:GLN:O	1:E:1877:ASN:ND2	2.28	0.60
1:C:1897:HIS:HE2	1:C:1961:SER:HB2	1.64	0.60
1:F:2096:ILE:HD12	1:F:2096:ILE:O	2.01	0.60
1:A:1020:ASP:OD1	1:A:1021:MET:N	2.35	0.60
1:D:2296:SER:O	1:D:2300:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1680:ILE:HG21	1:D:1699:PHE:HD1	1.67	0.60
1:D:2286:SER:O	1:D:2286:SER:OG	2.18	0.60
1:C:1700:LEU:CB	1:C:1803:ILE:HD11	2.31	0.60
1:A:1369:ILE:HA	1:A:1393:ALA:HB2	1.84	0.60
1:D:662:PRO:HG2	1:D:665:THR:HG23	1.83	0.60
1:D:1789:GLU:OE1	1:D:1792:ILE:HG23	2.02	0.60
1:E:2094:VAL:HG11	1:F:1827:ILE:HD13	1.83	0.60
1:D:2319:ILE:HD13	1:C:2319:ILE:HG23	1.84	0.60
1:E:1636:GLU:OE1	1:E:1636:GLU:N	2.35	0.60
1:B:926:ALA:O	1:B:929:ILE:HG22	2.02	0.60
1:D:1099:GLN:O	1:D:1102:SER:OG	2.15	0.60
1:E:2059:GLN:HE21	1:F:1878:ASN:HB2	1.66	0.60
1:A:638:HIS:NE2	1:A:725:THR:OG1	2.27	0.60
1:A:966:GLN:HA	1:A:969:VAL:HG12	1.84	0.60
1:E:1121:GLN:O	1:E:1125:LEU:HD23	2.01	0.59
1:A:1400:LYS:HG2	1:A:1426:ILE:HD11	1.84	0.59
1:D:1510:GLN:HE22	1:D:1512:GLU:HG3	1.66	0.59
1:D:1805:GLY:O	1:D:1808:SER:OG	2.15	0.59
1:D:892:PRO:O	1:D:925:TYR:OH	2.11	0.59
1:B:1020:ASP:OD1	1:B:1021:MET:N	2.35	0.59
1:D:898:GLU:O	1:D:902:ILE:HG22	2.02	0.59
1:D:1636:GLU:N	1:D:1636:GLU:OE1	2.35	0.59
1:D:2066:TYR:OH	1:C:1833:ARG:NH2	2.35	0.59
1:D:2289:GLU:N	1:D:2289:GLU:OE1	2.31	0.59
1:E:1099:GLN:O	1:E:1102:SER:OG	2.14	0.59
1:E:964:ASN:O	1:E:968:ILE:HG22	2.02	0.59
1:E:978:GLY:O	1:E:982:HIS:ND1	2.35	0.59
1:F:2021:ASP:OD1	1:F:2022:SER:N	2.35	0.59
1:A:898:GLU:OE1	1:A:975:TYR:OH	2.20	0.59
1:D:943:ASN:OD1	1:D:944:ILE:N	2.34	0.59
1:D:2059:GLN:HE21	1:C:1878:ASN:HB2	1.68	0.59
1:F:2085:GLN:N	1:F:2112:GLU:O	2.32	0.59
1:A:918:ILE:O	1:A:922:MET:HG2	2.02	0.59
1:A:929:ILE:O	1:A:930:THR:OG1	2.19	0.59
1:F:1534:ASN:ND2	1:F:1539:TYR:O	2.36	0.59
1:D:1445:GLU:O	1:D:1449:LEU:HD13	2.03	0.59
1:D:2249:ARG:NH1	1:E:953:ASN:OD1	2.36	0.59
1:E:1966:PRO:HA	1:E:1969:GLN:HE21	1.66	0.59
1:C:2021:ASP:OD1	1:C:2022:SER:N	2.36	0.59
1:C:2123:THR:HG21	1:C:2187:ALA:HB1	1.85	0.59
1:E:1518:ARG:NH1	1:E:1523:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:VAL:HG22	1:E:681:TYR:CE2	2.38	0.58
1:D:2240:THR:O	1:D:2244:ILE:HD12	2.03	0.58
1:E:2174:PHE:O	1:F:1745:TYR:OH	2.21	0.58
1:A:982:HIS:O	1:A:986:VAL:HG12	2.03	0.58
1:E:2057:TYR:OH	1:F:1877:ASN:O	2.20	0.58
1:E:2089:ARG:NH2	1:E:2188:ASP:OD1	2.36	0.58
1:B:923:ALA:O	1:B:926:ALA:HB3	2.03	0.58
1:E:2182:VAL:HG22	1:F:1748:TYR:CE1	2.39	0.58
1:F:2000:ASP:N	1:F:2006:SER:OG	2.34	0.58
1:A:1045:ILE:HD12	1:A:1046:ASP:N	2.18	0.58
1:D:1327:LEU:HD23	1:D:1358:PHE:O	2.04	0.58
1:D:1803:ILE:CD1	1:D:1831:LEU:HD11	2.31	0.58
1:E:1230:CYS:O	1:E:1232:ARG:NH1	2.36	0.58
1:F:2178:ILE:HD12	1:F:2181:GLN:HE21	1.69	0.58
1:D:1167:GLN:N	1:D:1167:GLN:OE1	2.36	0.58
1:B:918:ILE:O	1:B:922:MET:HG2	2.04	0.58
1:A:1324:ILE:HD12	1:A:1324:ILE:O	2.03	0.58
1:D:863:VAL:HG21	1:D:881:TRP:HZ3	1.68	0.57
1:E:1063:LEU:HD11	1:E:1081:ALA:O	2.03	0.57
1:E:1437:ALA:HB3	1:E:1481:VAL:CG2	2.34	0.57
1:D:1832:VAL:HG21	1:D:1838:THR:HG23	1.85	0.57
1:E:683:LEU:HD13	1:E:697:MET:HG2	1.85	0.57
1:C:1580:LYS:O	1:C:1583:LEU:N	2.37	0.57
1:C:1774:ASP:O	1:C:1779:ARG:NH1	2.37	0.57
1:A:1444:ASN:OD1	1:A:1445:GLU:N	2.36	0.57
1:D:1928:THR:OG1	1:D:1930:THR:O	2.19	0.57
1:F:1665:THR:OG1	1:F:1676:ASP:OD1	2.18	0.57
1:E:2319:ILE:O	1:E:2323:THR:N	2.37	0.57
1:C:2276:LYS:O	1:C:2277:GLN:NE2	2.37	0.57
1:F:1843:ASN:O	1:F:1843:ASN:ND2	2.34	0.57
1:D:1695:GLU:O	1:D:1698:LEU:HD23	2.04	0.57
1:E:1680:ILE:HG21	1:E:1699:PHE:HD1	1.70	0.57
1:E:2311:ASN:O	1:E:2314:VAL:HG12	2.04	0.57
1:F:1901:TYR:HB2	1:F:1902:MET:HE3	1.85	0.57
1:A:1069:LEU:CD1	1:A:1078:ALA:HB2	2.33	0.57
1:B:991:LEU:HD21	1:B:1066:LEU:HD21	1.86	0.57
1:E:1381:LEU:HD11	1:E:1426:ILE:HD11	1.87	0.57
1:C:2096:ILE:O	1:C:2096:ILE:HD12	2.04	0.57
1:C:2221:ARG:NH2	1:C:2264:TRP:O	2.35	0.57
1:F:1622:LEU:HD13	1:F:1669:PRO:HB3	1.87	0.57
1:E:1568:LEU:HD11	1:E:1571:MET:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:ALA:O	1:B:1416:VAL:HG12	2.04	0.57
1:D:1639:LEU:HD13	1:D:1640:ASP:O	2.05	0.57
1:E:1381:LEU:CD1	1:E:1426:ILE:HD11	2.35	0.57
1:E:1785:ILE:CD1	1:F:2189:LEU:HD13	2.35	0.57
1:E:2195:ARG:NE	1:F:1786:ILE:O	2.37	0.57
1:B:1408:ALA:HB2	1:B:1418:ASP:HB2	1.87	0.57
1:D:1748:TYR:CE1	1:C:2182:VAL:HG22	2.40	0.56
1:E:1886:CYS:N	1:E:1890:GLU:OE2	2.34	0.56
1:F:1480:THR:HG1	1:F:1518:ARG:HH12	1.53	0.56
1:F:1613:TRP:CZ3	1:F:1622:LEU:HD11	2.40	0.56
1:D:635:GLY:HA2	1:D:736:ILE:HD13	1.88	0.56
1:D:2062:LYS:HE2	1:C:1880:VAL:HG22	1.87	0.56
1:C:1858:LEU:HD13	1:C:1862:VAL:HG21	1.87	0.56
1:C:2082:ILE:HD12	1:C:2108:TYR:O	2.05	0.56
1:F:2026:THR:HG22	1:F:2030:ILE:HD12	1.88	0.56
1:A:1481:VAL:HG22	1:A:1515:ILE:HD11	1.87	0.56
1:E:852:VAL:O	1:E:856:VAL:HG23	2.04	0.56
1:E:2227:LEU:O	1:E:2230:LYS:HG2	2.05	0.56
1:C:1403:LEU:HB3	1:C:1423:VAL:HG23	1.88	0.56
1:C:1595:THR:OG1	1:C:1596:THR:N	2.39	0.56
1:D:1971:VAL:HG13	1:D:2025:LYS:NZ	2.20	0.56
1:A:955:LYS:O	1:A:956:SER:OG	2.19	0.56
1:D:636:ALA:HB2	1:D:683:LEU:HD22	1.86	0.56
1:D:1373:LEU:HD12	1:D:1402:HIS:HE1	1.71	0.56
1:E:1994:GLU:OE1	1:E:1994:GLU:N	2.39	0.56
1:C:1497:MET:SD	1:C:1498:ARG:N	2.78	0.56
1:F:1595:THR:OG1	1:F:1596:THR:N	2.38	0.56
1:B:1519:LEU:O	1:B:1523:GLY:N	2.35	0.56
1:D:1791:GLY:O	1:D:1796:ASN:ND2	2.39	0.56
1:D:1824:ALA:HB3	1:D:1846:LEU:HD13	1.87	0.56
1:C:2133:LEU:O	1:C:2136:THR:HG22	2.05	0.56
1:F:1861:GLU:OE2	1:F:1864:THR:HG22	2.05	0.56
1:F:2082:ILE:HD13	1:F:2109:ALA:HB2	1.86	0.56
1:A:1373:LEU:HG	1:A:1378:ALA:HB2	1.88	0.55
1:E:1815:ILE:HD11	1:E:2036:GLU:OE2	2.07	0.55
1:C:1727:ALA:HB3	1:C:1730:ILE:HG22	1.89	0.55
1:D:1568:LEU:O	1:D:1568:LEU:HD23	2.05	0.55
1:D:1718:ALA:HB2	1:D:1821:THR:HG22	1.88	0.55
1:D:1819:LEU:HD23	1:D:1819:LEU:H	1.70	0.55
1:E:938:SER:OG	1:E:939:GLN:N	2.39	0.55
1:C:1811:TYR:O	1:C:2035:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:ARG:NH2	1:A:1018:LYS:O	2.38	0.55
1:D:1785:ILE:CD1	1:C:2189:LEU:HD13	2.36	0.55
1:E:1785:ILE:HD11	1:F:2189:LEU:HD13	1.89	0.55
1:E:2124:VAL:HG13	1:E:2128:PHE:HB3	1.87	0.55
1:C:1680:ILE:HG21	1:C:1699:PHE:HD1	1.71	0.55
1:E:869:LEU:HD12	1:E:1036:LYS:HD2	1.88	0.55
1:C:1861:GLU:OE2	1:C:1864:THR:HG22	2.06	0.55
1:B:955:LYS:O	1:B:956:SER:OG	2.18	0.55
1:C:1956:ASP:OD1	1:C:2212:ARG:NH2	2.32	0.55
1:F:1565:GLN:NE2	1:F:1647:HIS:O	2.40	0.55
1:F:1858:LEU:HD13	1:F:1862:VAL:HG21	1.87	0.55
1:B:982:HIS:O	1:B:986:VAL:HG12	2.07	0.55
1:D:2124:VAL:HG13	1:D:2128:PHE:HB3	1.88	0.55
1:E:1707:ARG:HA	1:E:1814:ILE:HG21	1.88	0.55
1:B:1052:ASP:O	1:B:1054:THR:N	2.39	0.55
1:A:1069:LEU:HD13	1:A:1074:ASN:O	2.07	0.55
1:E:1000:GLN:CG	1:E:1013:LEU:HD23	2.37	0.55
1:C:1895:VAL:HG12	1:C:1899:LEU:HD12	1.89	0.55
1:C:2250:ARG:HD2	1:B:969:VAL:HG21	1.89	0.55
1:F:1995:LEU:N	1:F:2011:ILE:O	2.39	0.55
1:F:2186:PHE:HA	1:F:2189:LEU:HD12	1.88	0.55
1:D:1475:LEU:HD11	1:D:1477:PHE:CE1	2.42	0.54
1:D:1994:GLU:N	1:D:1994:GLU:OE1	2.40	0.54
1:B:1124:ILE:HD13	1:B:1159:ILE:HD12	1.89	0.54
1:D:1289:LEU:HD21	1:D:1291:VAL:HG13	1.87	0.54
1:D:1430:SER:O	1:D:1430:SER:OG	2.22	0.54
1:D:1829:ALA:O	1:D:1832:VAL:HG12	2.07	0.54
1:D:2311:ASN:O	1:D:2314:VAL:HG12	2.06	0.54
1:F:2034:ASN:HD21	1:F:2074:CYS:HA	1.72	0.54
1:D:1374:GLU:OE1	1:D:1377:LEU:N	2.35	0.54
1:D:1882:HIS:HA	1:D:1964:MET:HG2	1.89	0.54
1:E:1819:LEU:H	1:E:1819:LEU:HD23	1.71	0.54
1:B:686:THR:O	1:B:694:VAL:HG12	2.07	0.54
1:A:1045:ILE:HD13	1:A:1080:ARG:HD3	1.89	0.54
1:D:2057:TYR:OH	1:C:1877:ASN:O	2.22	0.54
1:E:1294:LYS:O	1:E:1295:THR:OG1	2.18	0.54
1:B:1063:LEU:HD13	1:B:1066:LEU:HD12	1.88	0.54
1:D:1797:LEU:HG	1:C:2094:VAL:HG22	1.90	0.54
1:D:1970:THR:HA	1:D:1989:GLU:HB3	1.90	0.54
1:B:1056:THR:OG1	1:B:1057:ASP:N	2.41	0.54
1:B:1544:LEU:O	1:B:1564:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1924:GLU:O	1:D:2209:LYS:NZ	2.41	0.54
1:F:2082:ILE:HD12	1:F:2108:TYR:O	2.07	0.54
1:A:1480:THR:HG1	1:A:1518:ARG:HH12	1.56	0.54
1:E:968:ILE:O	1:E:972:VAL:HG12	2.08	0.54
1:F:2325:HIS:O	1:F:2327:SER:N	2.41	0.54
1:E:1510:GLN:OE1	1:E:1577:TYR:OH	2.26	0.54
1:E:1971:VAL:HG13	1:E:2025:LYS:HZ2	1.73	0.54
1:E:2117:VAL:HG11	1:F:1722:ALA:HB3	1.90	0.54
1:F:1774:ASP:O	1:F:1779:ARG:NH1	2.41	0.54
1:A:1046:ASP:OD1	1:A:1047:GLN:N	2.40	0.54
1:D:1716:VAL:CG2	1:D:1819:LEU:HD21	2.35	0.54
1:E:864:MET:SD	1:E:990:LEU:HD13	2.48	0.54
1:C:2044:ALA:CB	1:C:2088:LEU:HD11	2.38	0.54
1:A:1034:VAL:O	1:A:1038:ASN:N	2.41	0.54
1:E:1083:GLN:OE1	1:E:1444:ASN:ND2	2.41	0.53
1:C:2325:HIS:O	1:C:2327:SER:N	2.41	0.53
1:D:1931:PRO:HB2	1:D:1991:ARG:HG2	1.90	0.53
1:E:884:ARG:O	1:E:888:THR:HG23	2.08	0.53
1:F:2319:ILE:HA	1:F:2322:MET:HB2	1.90	0.53
1:B:864:MET:CE	1:B:1040:LEU:HD22	2.39	0.53
1:D:703:GLU:OE1	1:D:877:LYS:NZ	2.41	0.53
1:D:2093:TRP:CD1	1:C:1797:LEU:HD22	2.43	0.53
1:F:1971:VAL:HG22	1:F:1988:VAL:HG22	1.91	0.53
1:F:2034:ASN:ND2	1:F:2074:CYS:HA	2.22	0.53
1:E:1471:ASN:ND2	1:E:1507:ARG:O	2.41	0.53
1:E:2057:TYR:O	1:F:1878:ASN:ND2	2.30	0.53
1:C:2022:SER:O	1:C:2026:THR:OG1	2.18	0.53
1:F:1539:TYR:HH	1:F:1606:ARG:NH1	2.06	0.53
1:B:1037:LYS:O	1:B:1041:VAL:HG23	2.09	0.53
1:E:1063:LEU:HD12	1:E:1085:LEU:CD1	2.36	0.53
1:E:1549:THR:HG23	1:E:1556:ILE:HD13	1.89	0.53
1:D:901:ASP:O	1:D:904:THR:OG1	2.24	0.53
1:D:2295:ILE:HA	1:E:939:GLN:HE22	1.74	0.53
1:A:686:THR:O	1:A:694:VAL:HG12	2.09	0.53
1:D:1688:ILE:O	1:D:1688:ILE:HG22	2.08	0.53
1:D:2264:TRP:O	1:D:2270:LEU:HD22	2.09	0.53
1:E:848:LYS:O	1:E:852:VAL:HG23	2.08	0.53
1:E:1928:THR:OG1	1:E:1930:THR:O	2.24	0.53
1:B:1039:LEU:O	1:B:1042:THR:OG1	2.11	0.53
1:A:1125:LEU:HD12	1:A:1125:LEU:O	2.08	0.53
1:D:1540:LEU:O	1:D:1540:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1671:TYR:OH	1:D:1904:LYS:N	2.37	0.53
1:E:920:LYS:O	1:E:923:ALA:HB3	2.08	0.53
1:E:1475:LEU:HD12	1:E:1475:LEU:O	2.08	0.53
1:E:1598:ILE:HD12	1:E:1660:VAL:HG21	1.89	0.53
1:B:1125:LEU:O	1:B:1125:LEU:HD12	2.09	0.53
1:A:1403:LEU:HD21	1:A:1456:GLU:HB3	1.90	0.53
1:D:1102:SER:OG	1:D:1103:ILE:N	2.41	0.53
1:D:2064:GLY:O	1:D:2067:ILE:HG22	2.09	0.53
1:E:965:THR:O	1:E:969:VAL:HG13	2.08	0.53
1:C:2319:ILE:HA	1:C:2322:MET:HB2	1.90	0.53
1:F:2087:GLU:O	1:F:2088:LEU:HD22	2.08	0.53
1:B:950:ALA:O	1:B:953:ASN:ND2	2.41	0.53
1:B:1294:LYS:O	1:B:1295:THR:OG1	2.23	0.53
1:D:1091:PRO:HB2	1:D:1095:LEU:HD21	1.90	0.53
1:D:1873:GLN:O	1:D:1877:ASN:ND2	2.33	0.53
1:E:1531:PHE:O	1:E:1543:SER:OG	2.20	0.53
1:E:1699:PHE:CD2	1:E:1803:ILE:HD11	2.44	0.53
1:E:1723:ARG:HD3	1:E:1792:ILE:HG22	1.91	0.53
1:E:1917:ASP:OD1	1:E:1921:ARG:NE	2.42	0.53
1:C:1995:LEU:N	1:C:2011:ILE:O	2.40	0.53
1:B:1132:ASP:OD1	1:B:1352:PHE:N	2.41	0.53
1:B:1391:LEU:O	1:B:1391:LEU:HD12	2.09	0.53
1:D:1886:CYS:N	1:D:1890:GLU:OE2	2.35	0.52
1:E:705:ASP:OD1	1:E:705:ASP:N	2.42	0.52
1:E:2057:TYR:HD1	1:F:1874:ILE:HG23	1.74	0.52
1:C:2026:THR:HG22	1:C:2030:ILE:HD12	1.90	0.52
1:C:2082:ILE:HG12	1:C:2088:LEU:HD12	1.89	0.52
1:B:1092:SER:O	1:B:1092:SER:OG	2.27	0.52
1:B:1175:THR:HG23	1:B:1237:VAL:HG13	1.91	0.52
1:D:661:LEU:O	1:D:1006:TYR:OH	2.27	0.52
1:E:863:VAL:HG21	1:E:881:TRP:HZ3	1.72	0.52
1:E:947:SER:O	1:E:950:ALA:HB3	2.09	0.52
1:C:2000:ASP:N	1:C:2006:SER:OG	2.34	0.52
1:C:2186:PHE:HA	1:C:2189:LEU:HD12	1.90	0.52
1:F:1403:LEU:HB3	1:F:1423:VAL:HG23	1.91	0.52
1:B:969:VAL:HA	1:B:972:VAL:HG12	1.90	0.52
1:A:1045:ILE:HG21	1:A:1080:ARG:NH2	2.24	0.52
1:A:1120:LEU:CD2	1:A:1155:ARG:HE	2.23	0.52
1:A:1331:VAL:HG22	1:A:1354:LYS:O	2.09	0.52
1:C:1839:ILE:HD12	1:C:1895:VAL:HG22	1.91	0.52
1:C:1941:ARG:O	1:C:1951:LEU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2111:ARG:HG2	1:F:2205:ILE:HG21	1.91	0.52
1:B:634:CYS:O	1:B:638:HIS:HB2	2.08	0.52
1:B:1045:ILE:HD11	1:B:1084:VAL:HG21	1.90	0.52
1:D:1418:ASP:OD1	1:D:1419:TYR:N	2.42	0.52
1:D:1923:ILE:HD11	1:D:2212:ARG:HB2	1.90	0.52
1:E:1728:GLU:OE1	1:E:1731:ARG:NH2	2.42	0.52
1:C:1828:GLY:O	1:C:1832:VAL:HG23	2.09	0.52
1:F:1991:ARG:NH1	1:F:1993:VAL:HG22	2.24	0.52
1:F:2132:ASP:O	1:F:2136:THR:HG23	2.08	0.52
1:B:674:LEU:HD13	1:B:734:TYR:CD2	2.44	0.52
1:D:1042:THR:HA	1:D:1045:ILE:HG13	1.91	0.52
1:D:2304:ILE:CD1	1:C:2304:ILE:HD12	2.39	0.52
1:E:901:ASP:O	1:E:904:THR:OG1	2.26	0.52
1:B:864:MET:HE2	1:B:1040:LEU:HD22	1.91	0.52
1:B:1390:ASP:N	1:B:1407:ALA:O	2.42	0.52
1:A:1006:TYR:O	1:A:1010:VAL:HG23	2.10	0.52
1:A:1167:GLN:N	1:A:1167:GLN:OE1	2.43	0.52
1:D:1978:LEU:HD11	1:D:2212:ARG:HG3	1.91	0.52
1:E:857:LEU:HD21	1:E:885:LEU:HD11	1.90	0.52
1:E:1784:ASP:OD2	1:F:2195:ARG:N	2.42	0.52
1:D:641:ASP:OD1	1:D:642:VAL:N	2.42	0.52
1:D:2057:TYR:HD1	1:C:1874:ILE:HG23	1.75	0.52
1:E:960:VAL:HG12	1:E:964:ASN:HD21	1.75	0.52
1:E:1682:ASN:HD21	1:E:1718:ALA:C	2.12	0.52
1:B:1482:ILE:HG23	1:B:1519:LEU:HD13	1.92	0.52
1:D:947:SER:O	1:D:950:ALA:HB3	2.10	0.52
1:E:1750:TYR:OH	1:E:1774:ASP:OD2	2.24	0.52
1:E:2173:GLU:HA	1:E:2176:ILE:HD12	1.91	0.52
1:F:1539:TYR:OH	1:F:1606:ARG:NH1	2.42	0.52
1:B:1301:ASP:OD1	1:B:1302:ASP:N	2.43	0.52
1:A:1079:LEU:HD21	1:A:1447:GLU:CB	2.40	0.52
1:E:2075:CYS:O	1:E:2104:HIS:NE2	2.43	0.52
1:C:1385:ARG:NH1	1:C:1512:GLU:OE2	2.42	0.52
1:F:2150:ARG:O	1:F:2156:LEU:HD11	2.09	0.52
1:A:1069:LEU:HD21	1:A:1077:VAL:HG12	1.92	0.52
1:D:1091:PRO:CB	1:D:1095:LEU:HD21	2.40	0.51
1:B:1014:ARG:NH2	1:B:1018:LYS:O	2.43	0.51
1:B:1178:VAL:HG12	1:B:1236:MET:CB	2.39	0.51
1:E:1290:ASN:OD1	1:E:1328:THR:OG1	2.16	0.51
1:B:997:VAL:HG22	1:B:1027:TYR:CZ	2.45	0.51
1:B:1181:GLN:NE2	1:B:1233:MET:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:THR:O	1:D:694:VAL:HG12	2.11	0.51
1:D:1499:TYR:CE1	1:D:1502:ARG:HB3	2.45	0.51
1:D:1534:ASN:ND2	1:D:1539:TYR:O	2.43	0.51
1:C:1568:LEU:HD23	1:C:1568:LEU:O	2.10	0.51
1:B:668:ASN:ND2	1:B:868:CYS:SG	2.83	0.51
1:A:1045:ILE:HG21	1:A:1080:ARG:CZ	2.40	0.51
1:D:2016:GLN:O	1:D:2047:ARG:N	2.41	0.51
1:E:1556:ILE:HB	1:E:1573:ILE:HD11	1.92	0.51
1:F:1973:VAL:HG12	1:F:1986:VAL:HG12	1.91	0.51
1:A:1556:ILE:HB	1:A:1573:ILE:HG21	1.91	0.51
1:E:1719:ASN:OD1	1:E:1720:SER:N	2.35	0.51
1:C:1640:ASP:OD1	1:C:1642:GLN:N	2.44	0.51
1:F:1828:GLY:O	1:F:1832:VAL:HG23	2.10	0.51
1:B:943:ASN:OD1	1:B:944:ILE:N	2.44	0.51
1:B:1014:ARG:O	1:B:1018:LYS:CA	2.57	0.51
1:D:965:THR:O	1:D:969:VAL:HG13	2.10	0.51
1:D:1101:GLU:O	1:D:1105:LEU:HD23	2.11	0.51
1:D:1684:ILE:HD12	1:D:1718:ALA:C	2.31	0.51
1:E:950:ALA:O	1:E:954:ARG:NH2	2.44	0.51
1:F:2064:GLY:O	1:F:2067:ILE:HG22	2.10	0.51
1:D:998:GLU:OE1	1:D:1074:ASN:ND2	2.42	0.51
1:D:2119:GLU:OE1	1:D:2121:GLU:N	2.43	0.51
1:E:1534:ASN:ND2	1:E:1539:TYR:O	2.44	0.51
1:C:2135:LYS:O	1:C:2138:ARG:NH1	2.44	0.51
1:F:2178:ILE:CD1	1:F:2181:GLN:HE21	2.23	0.51
1:A:1013:LEU:HD13	1:A:1024:VAL:HG13	1.92	0.51
1:A:1066:LEU:HD11	1:A:1080:ARG:HH22	1.75	0.51
1:E:2064:GLY:O	1:E:2067:ILE:HG22	2.11	0.51
1:E:2232:ILE:O	1:E:2235:ALA:HB3	2.11	0.51
1:E:2336:ARG:CG	1:E:2337:ILE:HD12	2.40	0.51
1:C:1454:MET:HG2	1:C:1506:LEU:HD21	1.93	0.51
1:F:1956:ASP:OD1	1:F:2212:ARG:NH2	2.36	0.51
1:D:935:GLN:OE1	1:D:935:GLN:N	2.44	0.51
1:D:1299:ILE:O	1:D:1301:ASP:N	2.42	0.51
1:B:992:ARG:HE	1:B:1062:ILE:HD11	1.76	0.51
1:B:1069:LEU:CD1	1:B:1078:ALA:HB2	2.41	0.51
1:B:1120:LEU:CD2	1:B:1155:ARG:HE	2.24	0.51
1:B:1241:THR:HG23	1:B:1244:ASP:H	1.75	0.51
1:D:1082:ARG:HA	1:D:1085:LEU:HD12	1.93	0.51
1:E:706:VAL:HG22	1:E:707:HIS:H	1.76	0.51
1:E:1101:GLU:O	1:E:1105:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1405:LEU:HD23	1:E:1421:PHE:CD1	2.46	0.51
1:F:1499:TYR:O	1:F:1503:LEU:HD13	2.10	0.51
1:F:1766:SER:O	1:F:1786:ILE:N	2.41	0.51
1:F:1999:ALA:HB2	1:F:2008:ALA:N	2.26	0.51
1:B:705:ASP:OD1	1:B:717:SER:OG	2.15	0.51
1:B:1386:MET:HE2	1:B:1391:LEU:HD23	1.92	0.51
1:E:1755:PRO:HA	1:E:1758:TYR:CD1	2.46	0.50
1:E:2322:MET:SD	1:F:2308:VAL:HG11	2.51	0.50
1:C:2144:TYR:CE1	1:C:2168:LEU:HD11	2.46	0.50
1:C:2236:ASN:ND2	1:C:2295:ILE:HG22	2.27	0.50
1:F:1895:VAL:HG12	1:F:1899:LEU:HD12	1.92	0.50
1:B:1140:HIS:O	1:B:1146:ARG:NH2	2.44	0.50
1:A:889:LEU:HD23	1:A:983:MET:HG2	1.93	0.50
1:D:1568:LEU:HD21	1:D:1571:MET:HG2	1.93	0.50
1:D:1837:ARG:NH2	1:D:2032:ASP:OD2	2.44	0.50
1:D:1981:ILE:HD12	1:D:1981:ILE:O	2.11	0.50
1:D:2045:ASN:HD21	1:D:2083:PRO:HD2	1.76	0.50
1:F:1897:HIS:HE2	1:F:1961:SER:HB2	1.76	0.50
1:F:2201:VAL:HG23	1:F:2202:ILE:HG23	1.92	0.50
1:E:968:ILE:CD1	1:E:971:LEU:HD23	2.42	0.50
1:E:1299:ILE:O	1:E:1301:ASP:N	2.41	0.50
1:E:2117:VAL:CG2	1:F:1797:LEU:HD21	2.41	0.50
1:A:1408:ALA:HB2	1:A:1418:ASP:HB2	1.93	0.50
1:D:1375:PRO:O	1:D:1379:PHE:HA	2.10	0.50
1:D:1680:ILE:HD13	1:D:1699:PHE:CD1	2.47	0.50
1:D:2232:ILE:O	1:D:2235:ALA:HB3	2.11	0.50
1:E:1517:ILE:HG12	1:E:1518:ARG:H	1.76	0.50
1:C:2007:GLU:O	1:C:2009:LYS:NZ	2.42	0.50
1:E:640:ALA:CB	1:E:685:VAL:HG11	2.42	0.50
1:E:1289:LEU:HD21	1:E:1291:VAL:HG13	1.93	0.50
1:C:2044:ALA:HB1	1:C:2088:LEU:HD11	1.92	0.50
1:C:2232:ILE:O	1:C:2235:ALA:HB3	2.12	0.50
1:B:1534:ASN:HD22	1:B:1535:GLU:N	2.09	0.50
1:A:943:ASN:OD1	1:A:944:ILE:N	2.45	0.50
1:D:1408:ALA:HB2	1:D:1418:ASP:CB	2.42	0.50
1:D:1750:TYR:OH	1:D:1774:ASP:OD2	2.27	0.50
1:E:2264:TRP:O	1:E:2270:LEU:HD11	2.12	0.50
1:C:1874:ILE:HG22	1:C:1875:MET:HE2	1.94	0.50
1:F:1839:ILE:HD12	1:F:1895:VAL:HG22	1.93	0.50
1:D:668:ASN:ND2	1:D:868:CYS:SG	2.85	0.50
1:E:1598:ILE:CD1	1:E:1660:VAL:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1805:GLY:O	1:E:1808:SER:OG	2.19	0.50
1:F:1568:LEU:HD23	1:F:1568:LEU:O	2.12	0.50
1:F:2224:LEU:CB	1:F:2274:LEU:HD13	2.41	0.50
1:F:2224:LEU:HB2	1:F:2274:LEU:HD13	1.93	0.50
1:A:1240:ARG:NH2	1:A:1244:ASP:OD2	2.45	0.50
1:F:1851:ALA:HB1	1:F:1863:TYR:CB	2.40	0.50
1:B:1086:ILE:O	1:B:1089:HIS:N	2.45	0.50
1:A:1288:ILE:O	1:A:1289:LEU:HD22	2.12	0.50
1:D:1622:LEU:H	1:D:1622:LEU:HD23	1.77	0.50
1:E:2322:MET:HG2	1:F:2308:VAL:HG11	1.93	0.50
1:A:648:VAL:HG22	1:A:666:LEU:HD11	1.93	0.50
1:A:950:ALA:O	1:A:953:ASN:ND2	2.44	0.50
1:A:1069:LEU:CD2	1:A:1077:VAL:HG12	2.42	0.50
1:C:1897:HIS:HE2	1:C:1961:SER:CB	2.25	0.49
1:C:1902:MET:SD	1:C:1902:MET:N	2.85	0.49
1:C:1999:ALA:HB2	1:C:2008:ALA:N	2.26	0.49
1:F:1555:GLN:HB3	1:F:1572:LEU:HD21	1.93	0.49
1:D:953:ASN:OD1	1:E:2249:ARG:NH1	2.45	0.49
1:E:1789:GLU:OE1	1:E:1792:ILE:HG23	2.12	0.49
1:E:2119:GLU:OE1	1:E:2121:GLU:N	2.44	0.49
1:B:1548:VAL:HG21	1:B:1559:GLN:OE1	2.12	0.49
1:D:899:LEU:HD13	1:D:922:MET:SD	2.52	0.49
1:E:727:MET:SD	1:E:727:MET:N	2.84	0.49
1:E:1102:SER:OG	1:E:1103:ILE:N	2.46	0.49
1:E:1289:LEU:HD22	1:E:1327:LEU:CD1	2.42	0.49
1:A:849:LEU:HD21	1:A:888:THR:HG22	1.94	0.49
1:D:1102:SER:O	1:D:1106:SER:OG	2.26	0.49
1:D:1774:ASP:O	1:D:1779:ARG:NH1	2.46	0.49
1:E:696:ILE:HG23	1:E:700:SER:O	2.12	0.49
1:C:2230:LYS:O	1:C:2234:ASN:ND2	2.46	0.49
1:A:1391:LEU:HD13	1:A:1404:TYR:CD2	2.48	0.49
1:D:1723:ARG:HG2	1:D:1792:ILE:HG22	1.95	0.49
1:E:1637:LEU:HB3	1:E:1645:LEU:HD11	1.93	0.49
1:C:1878:ASN:OD1	1:C:1880:VAL:HG23	2.13	0.49
1:B:1164:ASN:OD1	1:B:1164:ASN:N	2.46	0.49
1:D:1083:GLN:HG2	1:D:1444:ASN:HD22	1.76	0.49
1:D:2075:CYS:O	1:D:2104:HIS:NE2	2.46	0.49
1:E:640:ALA:O	1:E:644:LEU:HD13	2.13	0.49
1:E:1039:LEU:O	1:E:1042:THR:OG1	2.15	0.49
1:C:1705:LEU:O	1:C:1708:ALA:HB3	2.13	0.49
1:B:1006:TYR:O	1:B:1010:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2304:ILE:HD13	1:C:2304:ILE:HD12	1.93	0.49
1:E:1421:PHE:CE1	1:E:1460:ALA:HB1	2.47	0.49
1:E:1716:VAL:CG2	1:E:1819:LEU:HD21	2.37	0.49
1:F:1941:ARG:O	1:F:1951:LEU:N	2.43	0.49
1:B:1369:ILE:HA	1:B:1393:ALA:HB2	1.95	0.49
1:E:2078:VAL:CG1	1:E:2105:MET:HG2	2.43	0.49
1:E:2116:SER:OG	1:E:2191:ASP:OD2	2.27	0.49
1:C:2119:GLU:OE1	1:C:2121:GLU:N	2.46	0.49
1:B:1314:GLN:HE22	1:B:1315:ASN:ND2	2.10	0.49
1:E:1528:ILE:HD12	1:E:1530:LEU:HD11	1.95	0.49
1:E:1897:HIS:O	1:E:1900:SER:OG	2.19	0.49
1:E:2079:LEU:HD12	1:E:2079:LEU:O	2.12	0.49
1:B:1069:LEU:O	1:B:1069:LEU:HD12	2.12	0.49
1:A:1534:ASN:HD22	1:A:1535:GLU:N	2.10	0.49
1:D:1042:THR:HA	1:D:1045:ILE:CG1	2.42	0.49
1:F:2111:ARG:HG2	1:F:2205:ILE:CG2	2.43	0.49
1:A:1314:GLN:HE22	1:A:1315:ASN:ND2	2.11	0.49
1:D:913:ASN:OD1	1:D:913:ASN:N	2.46	0.48
1:D:1421:PHE:CZ	1:D:1460:ALA:HB1	2.48	0.48
1:D:1689:GLY:O	1:D:1719:ASN:ND2	2.46	0.48
1:D:2117:VAL:HG11	1:C:1722:ALA:HB3	1.95	0.48
1:E:1622:LEU:HD23	1:E:1622:LEU:H	1.77	0.48
1:C:2034:ASN:ND2	1:C:2074:CYS:HA	2.27	0.48
1:F:2119:GLU:OE1	1:F:2121:GLU:HG2	2.13	0.48
1:F:1558:PHE:CZ	1:F:1573:ILE:HD13	2.47	0.48
1:A:1124:ILE:HD13	1:A:1159:ILE:HD12	1.94	0.48
1:A:1130:ILE:HG22	1:A:1130:ILE:O	2.13	0.48
1:A:1298:ASP:H	1:A:1304:LEU:HD11	1.78	0.48
1:D:920:LYS:O	1:D:923:ALA:HB3	2.13	0.48
1:D:1309:ARG:O	1:D:1312:THR:OG1	2.21	0.48
1:E:2093:TRP:CD1	1:F:1797:LEU:HD22	2.48	0.48
1:C:1858:LEU:CD1	1:C:1862:VAL:HG21	2.44	0.48
1:B:992:ARG:HA	1:B:995:LEU:HB3	1.96	0.48
1:D:1664:MET:SD	1:D:1679:VAL:HG21	2.52	0.48
1:D:2117:VAL:HG23	1:C:1797:LEU:HD21	1.95	0.48
1:D:2239:LEU:HB2	1:D:2244:ILE:HD11	1.95	0.48
1:E:640:ALA:HB2	1:E:685:VAL:HG11	1.96	0.48
1:D:1785:ILE:HD11	1:C:2189:LEU:HD13	1.96	0.48
1:D:1925:PHE:O	1:D:2208:TRP:NE1	2.38	0.48
1:E:1923:ILE:HD13	1:E:1954:PHE:HA	1.94	0.48
1:C:1968:ALA:HB2	1:C:2021:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:ASP:OD1	1:A:1302:ASP:N	2.46	0.48
1:D:2221:ARG:NH2	1:D:2270:LEU:HD23	2.29	0.48
1:E:1115:PHE:CD1	1:E:1117:ILE:HD13	2.48	0.48
1:E:1931:PRO:HB2	1:E:1991:ARG:HG2	1.96	0.48
1:C:1470:CYS:HA	1:C:1509:LEU:HB3	1.95	0.48
1:D:1727:ALA:HB2	1:D:1787:GLY:HA2	1.94	0.48
1:E:1723:ARG:CD	1:E:1792:ILE:HG22	2.43	0.48
1:E:2333:GLU:O	1:E:2336:ARG:HG2	2.14	0.48
1:E:991:LEU:HD12	1:E:992:ARG:HE	1.79	0.48
1:F:1640:ASP:OD1	1:F:1642:GLN:N	2.47	0.48
1:F:2241:ASP:OD1	1:F:2242:GLY:N	2.46	0.48
1:B:947:SER:O	1:B:950:ALA:HB3	2.13	0.48
1:B:1386:MET:CE	1:B:1391:LEU:HD23	2.44	0.48
1:E:2079:LEU:HD13	1:E:2215:PHE:CE1	2.48	0.48
1:A:1436:GLU:N	1:A:1436:GLU:OE1	2.47	0.48
1:E:1528:ILE:HD12	1:E:1530:LEU:CD1	2.44	0.48
1:C:2064:GLY:O	1:C:2067:ILE:HG13	2.14	0.48
1:F:1874:ILE:HG22	1:F:1875:MET:HE2	1.96	0.48
1:F:2071:LEU:HD11	1:F:2105:MET:SD	2.54	0.48
1:F:2144:TYR:CE1	1:F:2168:LEU:HD11	2.49	0.48
1:A:641:ASP:HA	1:A:644:LEU:HD12	1.96	0.48
1:C:1499:TYR:O	1:C:1503:LEU:HD13	2.14	0.47
1:F:2110:ASP:O	1:F:2113:SER:OG	2.13	0.47
1:B:1386:MET:SD	1:B:1391:LEU:HD23	2.54	0.47
1:A:1108:ILE:HG13	1:A:1145:VAL:HG23	1.96	0.47
1:D:1707:ARG:HA	1:D:1814:ILE:HG21	1.95	0.47
1:D:1728:GLU:OE1	1:D:1732:HIS:NE2	2.47	0.47
1:C:1810:ALA:HB1	1:C:1814:ILE:HD11	1.96	0.47
1:C:1851:ALA:HB1	1:C:1863:TYR:CB	2.44	0.47
1:C:1865:SER:O	1:C:1868:GLN:HB2	2.14	0.47
1:F:1897:HIS:HE2	1:F:1961:SER:CB	2.27	0.47
1:B:1090:LEU:HD11	1:B:1096:ARG:NH1	2.29	0.47
1:A:991:LEU:HD21	1:A:1066:LEU:HD12	1.96	0.47
1:D:1130:ILE:O	1:D:1130:ILE:HG22	2.13	0.47
1:D:2055:ASP:OD1	1:D:2056:MET:N	2.47	0.47
1:E:1695:GLU:HA	1:E:1698:LEU:CD2	2.45	0.47
1:E:1791:GLY:O	1:E:1796:ASN:ND2	2.42	0.47
1:A:705:ASP:N	1:A:705:ASP:OD1	2.46	0.47
1:A:1288:ILE:C	1:A:1289:LEU:HD22	2.33	0.47
1:A:1480:THR:OG1	1:A:1480:THR:O	2.29	0.47
1:D:1919:ILE:O	1:D:2213:THR:OG1	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:668:ASN:OD1	1:E:687:ARG:NE	2.46	0.47
1:E:869:LEU:HD13	1:E:874:PHE:CD2	2.49	0.47
1:E:913:ASN:OD1	1:E:913:ASN:N	2.47	0.47
1:E:1786:ILE:O	1:F:2195:ARG:NE	2.47	0.47
1:F:1711:ILE:HG22	1:F:1905:SER:HB3	1.95	0.47
1:B:1059:LEU:HD13	1:B:1063:LEU:HD23	1.95	0.47
1:B:1373:LEU:HG	1:B:1378:ALA:HB2	1.96	0.47
1:A:1408:ALA:O	1:A:1416:VAL:HG12	2.13	0.47
1:A:1496:VAL:HG11	1:A:1540:LEU:CD1	2.44	0.47
1:D:955:LYS:O	1:D:956:SER:OG	2.23	0.47
1:D:2322:MET:SD	1:C:2308:VAL:HG11	2.54	0.47
1:E:1748:TYR:CD1	1:F:2182:VAL:HG22	2.49	0.47
1:C:1602:PRO:O	1:C:1605:PHE:HB3	2.15	0.47
1:A:851:ARG:O	1:A:855:TYR:HB3	2.14	0.47
1:D:1375:PRO:O	1:D:1379:PHE:CA	2.63	0.47
1:D:2057:TYR:O	1:C:1878:ASN:ND2	2.37	0.47
1:E:962:PHE:O	1:E:966:GLN:HB2	2.14	0.47
1:E:1083:GLN:HG2	1:E:1444:ASN:HD21	1.79	0.47
1:E:1392:THR:N	1:E:1405:LEU:O	2.43	0.47
1:C:1534:ASN:HD22	1:C:1535:GLU:N	2.13	0.47
1:C:2123:THR:HG21	1:C:2187:ALA:CB	2.44	0.47
1:F:1468:THR:O	1:F:1507:ARG:NH2	2.41	0.47
1:F:1602:PRO:O	1:F:1605:PHE:HB3	2.15	0.47
1:F:1705:LEU:O	1:F:1708:ALA:HB3	2.13	0.47
1:B:1154:VAL:HG13	1:B:1180:PHE:CE1	2.49	0.47
1:B:1314:GLN:HE22	1:B:1315:ASN:HD22	1.63	0.47
1:A:919:LYS:HA	1:A:922:MET:HG2	1.97	0.47
1:D:1517:ILE:HG12	1:D:1518:ARG:H	1.78	0.47
1:D:2284:VAL:O	1:D:2284:VAL:HG22	2.14	0.47
1:C:2207:ASP:OD1	1:C:2210:THR:OG1	2.32	0.47
1:F:1826:GLY:HA2	1:F:1848:LEU:HD23	1.96	0.47
1:F:2221:ARG:NH1	1:F:2266:ASN:O	2.47	0.47
1:B:1373:LEU:HD11	1:B:1378:ALA:HB2	1.95	0.47
1:A:636:ALA:HB1	1:A:685:VAL:HG22	1.95	0.47
1:A:1075:ALA:O	1:A:1079:LEU:HD13	2.14	0.47
1:D:1000:GLN:HE21	1:D:1016:GLU:CG	2.27	0.47
1:D:1734:PHE:O	1:C:2139:ARG:NE	2.48	0.47
1:E:943:ASN:OD1	1:E:944:ILE:N	2.47	0.47
1:E:1939:ALA:HB2	1:E:1960:PHE:HB3	1.97	0.47
1:F:1865:SER:O	1:F:1868:GLN:HB2	2.15	0.47
1:B:641:ASP:HA	1:B:644:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:PHE:HB2	1:B:1234:GLY:HA3	1.97	0.47
1:A:922:MET:HG3	1:A:923:ALA:N	2.30	0.47
1:A:1059:LEU:HD13	1:A:1063:LEU:HD23	1.96	0.47
1:F:2133:LEU:O	1:F:2136:THR:OG1	2.25	0.47
1:A:1481:VAL:CG2	1:A:1515:ILE:HD11	2.45	0.47
1:D:852:VAL:O	1:D:856:VAL:HG23	2.14	0.47
1:D:1530:LEU:HD12	1:D:1543:SER:O	2.15	0.47
1:E:1896:LEU:HD23	1:E:1899:LEU:HD12	1.97	0.47
1:E:2307:LEU:HD22	1:F:2304:ILE:HD11	1.97	0.47
1:D:663:ALA:HB1	1:D:1032:ALA:HB1	1.97	0.46
1:D:2182:VAL:HG22	1:C:1748:TYR:CE1	2.51	0.46
1:E:1130:ILE:HG22	1:E:1130:ILE:O	2.15	0.46
1:E:2295:ILE:HD12	1:E:2295:ILE:H	1.79	0.46
1:B:1240:ARG:O	1:B:1294:LYS:HB3	2.15	0.46
1:D:892:PRO:HG2	1:D:929:ILE:HD11	1.96	0.46
1:D:964:ASN:O	1:D:968:ILE:HD12	2.16	0.46
1:D:2076:GLN:HB3	1:D:2077:PRO:CD	2.46	0.46
1:E:892:PRO:HG2	1:E:929:ILE:HD11	1.96	0.46
1:E:1970:THR:HA	1:E:1989:GLU:HB3	1.98	0.46
1:A:696:ILE:HD11	1:A:870:PRO:CB	2.45	0.46
1:D:1243:GLU:O	1:D:1247:ARG:NE	2.47	0.46
1:D:1931:PRO:HB2	1:D:1991:ARG:CG	2.45	0.46
1:D:2201:VAL:HG23	1:D:2202:ILE:HG23	1.98	0.46
1:E:2284:VAL:HG22	1:E:2284:VAL:O	2.14	0.46
1:C:1874:ILE:HG22	1:C:1875:MET:CE	2.45	0.46
1:C:1971:VAL:HG22	1:C:1988:VAL:HG13	1.97	0.46
1:C:1973:VAL:HG12	1:C:1986:VAL:HG12	1.96	0.46
1:F:1874:ILE:HG22	1:F:1875:MET:CE	2.45	0.46
1:B:964:ASN:O	1:B:968:ILE:HG22	2.15	0.46
1:B:978:GLY:O	1:B:981:GLY:N	2.49	0.46
1:B:1097:HIS:HA	1:B:1100:VAL:HG22	1.97	0.46
1:A:1120:LEU:O	1:A:1124:ILE:HG13	2.15	0.46
1:A:1314:GLN:HE22	1:A:1315:ASN:HD22	1.62	0.46
1:A:1524:LYS:HD3	1:A:1526:ILE:HD11	1.97	0.46
1:D:990:LEU:HD13	1:D:1044:LEU:HD11	1.96	0.46
1:D:1981:ILE:HD12	1:D:1983:VAL:HG13	1.97	0.46
1:D:2228:VAL:O	1:D:2231:LYS:N	2.48	0.46
1:E:969:VAL:HA	1:E:972:VAL:HG12	1.97	0.46
1:E:1977:ARG:HD3	1:E:1980:GLY:HA2	1.98	0.46
1:C:1901:TYR:HB2	1:C:1902:MET:CE	2.46	0.46
1:C:2150:ARG:O	1:C:2156:LEU:HD11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2221:ARG:NH1	1:C:2266:ASN:O	2.49	0.46
1:F:1612:LEU:HD22	1:F:1896:LEU:CD1	2.38	0.46
1:E:1052:ASP:O	1:E:1054:THR:N	2.48	0.46
1:E:1102:SER:O	1:E:1106:SER:CB	2.63	0.46
1:E:1108:ILE:HG21	1:E:1144:VAL:CG1	2.45	0.46
1:F:1858:LEU:CD1	1:F:1862:VAL:HG21	2.44	0.46
1:B:878:VAL:HG21	1:B:1040:LEU:HD12	1.98	0.46
1:B:1120:LEU:O	1:B:1124:ILE:HG13	2.15	0.46
1:A:644:LEU:HD22	1:A:687:ARG:HD3	1.97	0.46
1:E:1028:ILE:HA	1:E:1031:HIS:CD2	2.50	0.46
1:C:2016:GLN:HE21	1:C:2045:ASN:ND2	2.08	0.46
1:B:1045:ILE:CD1	1:B:1084:VAL:HG21	2.45	0.46
1:D:2068:VAL:CG2	1:D:2095:VAL:HG12	2.45	0.46
1:D:2076:GLN:HB3	1:D:2077:PRO:HD2	1.98	0.46
1:E:859:ASN:O	1:E:863:VAL:HG23	2.16	0.46
1:E:1165:SER:HB2	1:E:1181:GLN:HG3	1.98	0.46
1:E:1751:LEU:O	1:E:1782:ILE:HG22	2.16	0.46
1:E:2320:ILE:HA	1:E:2323:THR:HG22	1.98	0.46
1:B:705:ASP:OD1	1:B:705:ASP:N	2.49	0.46
1:A:1037:LYS:O	1:A:1041:VAL:HG23	2.15	0.46
1:E:1094:GLU:HA	1:E:1097:HIS:HB3	1.98	0.46
1:E:2055:ASP:OD1	1:E:2056:MET:N	2.48	0.46
1:C:1480:THR:OG1	1:C:1480:THR:O	2.34	0.46
1:F:1971:VAL:HG22	1:F:1988:VAL:HG13	1.98	0.46
1:A:1309:ARG:NH1	1:A:1366:GLU:OE2	2.49	0.46
1:D:884:ARG:O	1:D:888:THR:HG23	2.16	0.46
1:E:2322:MET:CG	1:F:2308:VAL:HG11	2.46	0.46
1:C:1494:SER:HA	1:C:1497:MET:HG3	1.98	0.46
1:C:1705:LEU:O	1:C:1708:ALA:N	2.49	0.46
1:C:1753:LEU:HD11	1:C:1757:ASP:HB2	1.98	0.46
1:C:1860:ARG:HH21	1:C:2004:LEU:HD21	1.80	0.46
1:C:2090:GLY:O	1:C:2094:VAL:HG23	2.16	0.46
1:F:1424:ARG:HG2	1:F:1474:PHE:HB3	1.98	0.46
1:F:1580:LYS:O	1:F:1583:LEU:N	2.49	0.46
1:F:2080:VAL:HB	1:F:2107:MET:HG2	1.97	0.46
1:B:696:ILE:HD11	1:B:870:PRO:HB2	1.98	0.46
1:B:995:LEU:HD12	1:B:1066:LEU:HD23	1.97	0.46
1:A:1248:ILE:HG22	1:A:1248:ILE:O	2.15	0.46
1:D:638:HIS:CD2	1:D:736:ILE:HG23	2.51	0.46
1:D:1535:GLU:N	1:D:1535:GLU:OE1	2.49	0.46
1:A:963:MET:HG3	1:A:966:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:ASN:O	1:A:968:ILE:HG22	2.16	0.46
1:D:1530:LEU:HD11	1:D:1542:ILE:HG23	1.98	0.45
1:D:1695:GLU:HA	1:D:1698:LEU:CD2	2.46	0.45
1:C:1671:TYR:OH	1:C:1903:PRO:HA	2.16	0.45
1:B:1389:PHE:CD1	1:B:1408:ALA:HA	2.51	0.45
1:A:945:LEU:HD11	1:A:968:ILE:HD13	1.98	0.45
1:D:865:ASN:O	1:D:1030:SER:OG	2.28	0.45
1:D:952:LEU:HD11	1:D:957:GLU:HB2	1.98	0.45
1:D:1421:PHE:CD2	1:D:1457:LEU:HD12	2.51	0.45
1:D:2326:ILE:HG22	1:D:2327:SER:N	2.31	0.45
1:B:869:LEU:HD12	1:B:1036:LYS:HG3	1.98	0.45
1:D:1679:VAL:HG22	1:D:1714:ILE:CD1	2.38	0.45
1:E:2328:PRO:HA	1:E:2331:ARG:HG3	1.99	0.45
1:C:2067:ILE:HD12	1:C:2068:VAL:N	2.31	0.45
1:D:969:VAL:HA	1:D:972:VAL:HG12	1.99	0.45
1:D:1639:LEU:HD21	1:D:1643:GLY:HA2	1.99	0.45
1:D:1730:ILE:HD11	1:D:1761:VAL:HG11	1.98	0.45
1:D:2337:ILE:CG2	1:E:932:VAL:HG21	2.47	0.45
1:E:1236:MET:CE	1:E:1292:ALA:HB2	2.47	0.45
1:E:1475:LEU:HD13	1:E:1477:PHE:CE1	2.51	0.45
1:C:1568:LEU:HD21	1:C:1571:MET:HB2	1.97	0.45
1:C:1622:LEU:HD11	1:C:1669:PRO:HB3	1.99	0.45
1:F:1809:LEU:HD12	1:F:1810:ALA:N	2.31	0.45
1:B:1471:ASN:ND2	1:B:1506:LEU:O	2.48	0.45
1:D:1939:ALA:HB2	1:D:1960:PHE:CB	2.46	0.45
1:D:2221:ARG:NE	1:D:2267:ASN:O	2.49	0.45
1:E:2326:ILE:HG22	1:E:2327:SER:N	2.32	0.45
1:B:930:THR:O	1:B:930:THR:HG22	2.17	0.45
1:B:1024:VAL:O	1:B:1027:TYR:HB2	2.16	0.45
1:A:1066:LEU:HD22	1:A:1081:ALA:HB2	1.98	0.45
1:D:1095:LEU:HD22	1:D:1096:ARG:N	2.31	0.45
1:D:1526:ILE:CD1	1:D:1528:ILE:HD11	2.46	0.45
1:E:1689:GLY:O	1:E:1719:ASN:ND2	2.49	0.45
1:E:2326:ILE:HG22	1:E:2327:SER:H	1.82	0.45
1:C:2040:LEU:HB2	1:C:2078:VAL:HG22	1.99	0.45
1:F:1812:ASN:HA	1:F:2035:ARG:NH1	2.32	0.45
1:B:1248:ILE:O	1:B:1248:ILE:HG22	2.16	0.45
1:B:1369:ILE:HD12	1:B:1391:LEU:HD13	1.98	0.45
1:A:992:ARG:HE	1:A:1062:ILE:HD11	1.81	0.45
1:D:1475:LEU:HD11	1:D:1477:PHE:CG	2.52	0.45
1:D:2116:SER:OG	1:D:2191:ASP:OD2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2016:GLN:HE21	1:F:2045:ASN:ND2	2.14	0.45
1:B:696:ILE:HD11	1:B:870:PRO:CB	2.47	0.45
1:A:879:LYS:HA	1:A:1043:MET:HE1	1.98	0.45
1:A:1154:VAL:HG13	1:A:1180:PHE:CE1	2.52	0.45
1:D:1971:VAL:HG13	1:D:2025:LYS:HZ3	1.79	0.45
1:E:1816:THR:HG21	1:E:1835:GLY:HA2	1.98	0.45
1:E:2319:ILE:HD13	1:F:2319:ILE:HG23	1.99	0.45
1:F:1671:TYR:OH	1:F:1903:PRO:HA	2.16	0.45
1:F:1860:ARG:HH21	1:F:2004:LEU:HD21	1.81	0.45
1:B:1085:LEU:HD23	1:B:1085:LEU:O	2.17	0.45
1:D:625:ARG:HB3	1:D:626:PRO:CD	2.46	0.45
1:D:853:PHE:CZ	1:D:889:LEU:HD23	2.51	0.45
1:D:991:LEU:HD11	1:D:1062:ILE:HG21	1.99	0.45
1:D:1499:TYR:HD2	1:D:1503:LEU:HD22	1.80	0.45
1:D:1664:MET:HE3	1:D:1679:VAL:HG21	1.98	0.45
1:E:874:PHE:O	1:E:877:LYS:N	2.50	0.45
1:E:1178:VAL:HG12	1:E:1236:MET:HB3	1.98	0.45
1:E:1391:LEU:HD13	1:E:1391:LEU:H	1.82	0.45
1:F:1705:LEU:O	1:F:1708:ALA:N	2.49	0.45
1:B:1169:ARG:HB2	1:B:1177:VAL:HB	1.98	0.45
1:A:636:ALA:HB1	1:A:685:VAL:CG2	2.47	0.45
1:A:675:ILE:HD12	1:A:748:GLU:HB2	1.99	0.45
1:A:1180:PHE:O	1:A:1233:MET:HA	2.17	0.45
1:A:1389:PHE:HD1	1:A:1408:ALA:HA	1.82	0.45
1:D:1420:ARG:HE	1:D:1470:CYS:HB3	1.82	0.45
1:E:636:ALA:HB2	1:E:683:LEU:HG	1.99	0.45
1:E:1182:PHE:O	1:E:1231:GLN:HG3	2.17	0.45
1:E:1359:ARG:NH2	1:E:1367:ASP:OD2	2.49	0.45
1:C:1421:PHE:CE1	1:C:1460:ALA:HB1	2.52	0.45
1:B:922:MET:HG3	1:B:923:ALA:N	2.33	0.45
1:D:2239:LEU:CB	1:D:2244:ILE:HD11	2.48	0.44
1:E:871:ASP:HB3	1:E:872:PRO:HD2	1.99	0.44
1:C:1391:LEU:HD12	1:C:1391:LEU:O	2.17	0.44
1:F:1391:LEU:HD12	1:F:1391:LEU:O	2.16	0.44
1:B:1167:GLN:N	1:B:1167:GLN:OE1	2.50	0.44
1:A:1129:SER:HB2	1:A:1428:ARG:HE	1.81	0.44
1:A:1135:PRO:HA	1:A:1138:PHE:CD1	2.51	0.44
1:D:1917:ASP:OD1	1:D:1921:ARG:NE	2.46	0.44
1:F:2007:GLU:O	1:F:2009:LYS:NZ	2.45	0.44
1:A:1034:VAL:HB	1:A:1073:THR:HG21	1.98	0.44
1:D:1378:ALA:O	1:D:1381:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1970:THR:O	1:D:1970:THR:HG22	2.17	0.44
1:D:2239:LEU:HD23	1:D:2243:GLN:HE21	1.82	0.44
1:D:2335:ILE:HG23	1:C:2335:ILE:HG12	2.00	0.44
1:E:2239:LEU:HD23	1:E:2243:GLN:NE2	2.32	0.44
1:C:2319:ILE:O	1:C:2322:MET:HB2	2.17	0.44
1:F:2141:ASP:OD1	1:F:2171:ARG:NH2	2.50	0.44
1:B:625:ARG:HB3	1:B:626:PRO:CD	2.47	0.44
1:A:696:ILE:HD11	1:A:870:PRO:HB2	2.00	0.44
1:A:1468:THR:O	1:A:1507:ARG:NH2	2.47	0.44
1:D:938:SER:OG	1:D:939:GLN:N	2.51	0.44
1:D:1138:PHE:HB3	1:D:1149:ALA:HB3	1.99	0.44
1:D:1373:LEU:HD23	1:D:1373:LEU:HA	1.91	0.44
1:D:1939:ALA:HB2	1:D:1960:PHE:HB3	1.98	0.44
1:D:2097:ASP:O	1:D:2100:ILE:HD12	2.17	0.44
1:E:1114:GLN:NE2	1:E:1148:ALA:HB2	2.29	0.44
1:F:2046:TRP:HE3	1:F:2088:LEU:HD11	1.82	0.44
1:B:648:VAL:HG22	1:B:666:LEU:HD11	1.99	0.44
1:B:1082:ARG:HH22	1:B:1085:LEU:HD22	1.83	0.44
1:D:878:VAL:O	1:D:882:VAL:HG23	2.17	0.44
1:D:1817:ILE:HG12	1:D:1837:ARG:HD2	1.98	0.44
1:E:1436:GLU:N	1:E:1482:ILE:O	2.51	0.44
1:E:1443:GLN:HE22	1:E:1495:MET:HB2	1.81	0.44
1:E:2251:TRP:HA	1:E:2254:GLU:HG2	1.99	0.44
1:C:1753:LEU:HD11	1:C:1757:ASP:CB	2.48	0.44
1:C:1945:THR:O	1:C:1947:LYS:N	2.50	0.44
1:F:1878:ASN:OD1	1:F:1880:VAL:HG23	2.18	0.44
1:A:899:LEU:HD12	1:A:903:MET:HG2	1.98	0.44
1:A:1482:ILE:HG23	1:A:1519:LEU:HA	2.00	0.44
1:E:2054:LYS:HD2	1:F:2000:ASP:HB2	2.00	0.44
1:E:2059:GLN:NE2	1:F:1878:ASN:O	2.50	0.44
1:C:1709:GLU:O	1:C:1711:ILE:HD12	2.16	0.44
1:F:1394:ILE:HB	1:F:1403:LEU:HD12	1.99	0.44
1:B:1165:SER:HB2	1:B:1181:GLN:HG3	2.00	0.44
1:A:625:ARG:HB3	1:A:626:PRO:CD	2.46	0.44
1:D:1368:ARG:HA	1:D:1371:ARG:HG2	2.00	0.44
1:E:1753:LEU:HD22	1:E:1757:ASP:HB3	1.99	0.44
1:E:2288:ILE:HD12	1:E:2288:ILE:H	1.81	0.44
1:C:1421:PHE:CE2	1:C:1468:THR:HG21	2.53	0.44
1:F:1968:ALA:HB2	1:F:2021:ASP:HB2	2.00	0.44
1:F:2251:TRP:CD2	1:F:2288:ILE:HD11	2.53	0.44
1:B:990:LEU:O	1:B:993:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:997:VAL:HG13	1:B:1027:TYR:CG	2.52	0.44
1:A:849:LEU:HD21	1:A:888:THR:CG2	2.48	0.44
1:D:899:LEU:HA	1:D:902:ILE:HG22	1.99	0.44
1:E:625:ARG:HB3	1:E:626:PRO:CD	2.48	0.44
1:E:2068:VAL:HG21	1:E:2095:VAL:HG12	2.00	0.44
1:C:1705:LEU:HD13	1:C:1705:LEU:C	2.39	0.44
1:B:899:LEU:HD12	1:B:903:MET:HG2	1.99	0.44
1:A:1165:SER:HB2	1:A:1181:GLN:HG3	1.99	0.44
1:A:1410:VAL:HG12	1:A:1411:GLU:N	2.33	0.44
1:D:1736:VAL:HG22	1:D:1751:LEU:CD2	2.48	0.44
1:E:936:PHE:HE2	1:E:972:VAL:HG23	1.83	0.44
1:E:1680:ILE:HG21	1:E:1699:PHE:CD1	2.50	0.44
1:E:2196:MET:O	1:E:2201:VAL:HG22	2.18	0.44
1:C:2082:ILE:HD12	1:C:2082:ILE:H	1.83	0.44
1:C:2082:ILE:HD13	1:C:2109:ALA:HB2	1.98	0.44
1:C:2108:TYR:HB3	1:C:2206:LEU:HD13	1.99	0.44
1:F:2119:GLU:OE2	1:F:2122:GLY:N	2.51	0.44
1:A:992:ARG:O	1:A:996:ARG:HB3	2.18	0.44
1:A:993:GLN:O	1:A:997:VAL:HG23	2.18	0.44
1:A:1101:GLU:O	1:A:1105:LEU:HD23	2.18	0.44
1:E:919:LYS:HG2	1:E:922:MET:SD	2.58	0.43
1:E:1055:LEU:HD12	1:E:1059:LEU:HD13	2.00	0.43
1:E:1418:ASP:OD2	1:E:1420:ARG:HD2	2.17	0.43
1:E:1420:ARG:HG2	1:E:1470:CYS:HB3	1.98	0.43
1:E:1902:MET:HB3	1:E:2036:GLU:OE2	2.17	0.43
1:E:1960:PHE:HD1	1:E:1976:ALA:HB2	1.83	0.43
1:E:2117:VAL:HG22	1:F:1797:LEU:HD21	2.00	0.43
1:B:1154:VAL:CG2	1:B:1178:VAL:HG11	2.48	0.43
1:D:1178:VAL:HG12	1:D:1236:MET:HB2	1.99	0.43
1:D:1499:TYR:CE2	1:D:1503:LEU:HA	2.53	0.43
1:D:1892:VAL:HA	1:D:1895:VAL:HG12	1.99	0.43
1:E:899:LEU:HA	1:E:902:ILE:HG22	2.00	0.43
1:E:1627:LEU:N	1:E:1630:ASP:OD1	2.52	0.43
1:E:1923:ILE:CD1	1:E:2212:ARG:HB2	2.45	0.43
1:E:2236:ASN:HB3	1:E:2239:LEU:HD12	2.00	0.43
1:E:2329:THR:O	1:E:2332:ALA:HB3	2.18	0.43
1:F:1381:LEU:HB2	1:F:1383:LEU:HD23	2.00	0.43
1:A:1492:VAL:O	1:A:1496:VAL:HG12	2.18	0.43
1:D:950:ALA:O	1:D:954:ARG:NH2	2.51	0.43
1:D:1000:GLN:HE21	1:D:1016:GLU:HG3	1.83	0.43
1:D:1798:ARG:HB2	1:C:2201:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1819:LEU:HD23	1:D:1819:LEU:N	2.33	0.43
1:E:632:VAL:HG12	1:E:683:LEU:HD11	1.99	0.43
1:E:1180:PHE:HB2	1:E:1234:GLY:CA	2.47	0.43
1:C:2130:ARG:O	1:C:2133:LEU:N	2.51	0.43
1:F:1493:ARG:HD2	1:F:1542:ILE:HD11	2.00	0.43
1:A:969:VAL:HA	1:A:972:VAL:HG12	2.01	0.43
1:D:992:ARG:HA	1:D:995:LEU:HB3	2.01	0.43
1:D:1728:GLU:OE1	1:D:1731:ARG:NH2	2.51	0.43
1:D:2054:LYS:HD2	1:C:2000:ASP:HB2	2.00	0.43
1:E:1180:PHE:HB2	1:E:1234:GLY:HA3	2.00	0.43
1:E:1645:LEU:HD23	1:E:1705:LEU:HD22	2.00	0.43
1:C:1934:PRO:O	1:C:1937:MET:HG3	2.19	0.43
1:B:952:LEU:HD23	1:B:961:PHE:CD2	2.53	0.43
1:A:864:MET:CE	1:A:1040:LEU:HD22	2.48	0.43
1:D:705:ASP:N	1:D:705:ASP:OD1	2.49	0.43
1:D:995:LEU:HD22	1:D:1066:LEU:HD21	1.98	0.43
1:E:930:THR:HG22	1:E:930:THR:O	2.19	0.43
1:E:968:ILE:HD12	1:E:971:LEU:HD23	1.99	0.43
1:E:1632:LEU:HD12	1:E:1632:LEU:C	2.39	0.43
1:E:2068:VAL:CG2	1:E:2095:VAL:HG12	2.47	0.43
1:C:2251:TRP:CD2	1:C:2288:ILE:HD11	2.54	0.43
1:B:1175:THR:HG23	1:B:1239:PHE:CE1	2.53	0.43
1:D:1063:LEU:CD1	1:D:1081:ALA:HB1	2.49	0.43
1:D:1924:GLU:N	1:D:1952:SER:OG	2.41	0.43
1:D:2074:CYS:O	1:D:2101:ASN:ND2	2.52	0.43
1:C:1925:PHE:CD2	1:C:1937:MET:HA	2.54	0.43
1:F:1480:THR:OG1	1:F:1480:THR:O	2.35	0.43
1:F:2030:ILE:HG23	1:F:2040:LEU:HD13	2.00	0.43
1:F:2115:GLY:HA3	1:F:2196:MET:CE	2.49	0.43
1:F:2276:LYS:O	1:F:2277:GLN:NE2	2.52	0.43
1:B:638:HIS:CG	1:B:727:MET:HG3	2.53	0.43
1:B:1069:LEU:HD13	1:B:1074:ASN:O	2.19	0.43
1:B:1400:LYS:HG2	1:B:1426:ILE:HD11	1.99	0.43
1:A:1316:LYS:O	1:A:1319:LEU:N	2.51	0.43
1:D:990:LEU:HA	1:D:993:GLN:OE1	2.18	0.43
1:D:1164:ASN:OD1	1:D:1164:ASN:N	2.52	0.43
1:D:1528:ILE:HG23	1:D:1545:TYR:O	2.19	0.43
1:D:1812:ASN:OD1	1:D:2035:ARG:NH1	2.51	0.43
1:D:1923:ILE:HD13	1:D:1954:PHE:HA	2.00	0.43
1:E:1289:LEU:HD22	1:E:1327:LEU:HD13	2.00	0.43
1:E:1471:ASN:HD22	1:E:1507:ARG:C	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2319:ILE:O	1:F:2322:MET:HB2	2.19	0.43
1:B:1002:GLN:HG3	1:B:1002:GLN:O	2.17	0.43
1:B:1049:CYS:SG	1:B:1084:VAL:HG22	2.58	0.43
1:A:1078:ALA:O	1:A:1081:ALA:HB3	2.19	0.43
1:A:1139:TYR:HB3	1:A:1238:SER:OG	2.18	0.43
1:D:1133:VAL:O	1:D:1136:ASN:N	2.49	0.43
1:D:2325:HIS:O	1:D:2326:ILE:HD13	2.19	0.43
1:E:1585:SER:O	1:E:1589:GLN:NE2	2.52	0.43
1:E:1659:MET:HB3	1:E:1698:LEU:HD21	2.00	0.43
1:E:1978:LEU:O	1:E:1981:ILE:HD12	2.19	0.43
1:C:1493:ARG:CZ	1:C:1542:ILE:HD12	2.49	0.43
1:C:1499:TYR:HB3	1:C:1502:ARG:HB3	2.00	0.43
1:C:1597:TYR:O	1:C:1601:ILE:HD12	2.19	0.43
1:C:2041:MET:CE	1:C:2079:LEU:HD12	2.48	0.43
1:F:1791:GLY:C	1:F:1796:ASN:HD21	2.22	0.43
1:F:2108:TYR:HB3	1:F:2206:LEU:HD23	2.00	0.43
1:B:1410:VAL:HG12	1:B:1411:GLU:N	2.34	0.43
1:A:663:ALA:HB2	1:A:1028:ILE:HG22	2.01	0.43
1:A:1175:THR:HG23	1:A:1237:VAL:HG13	2.01	0.43
1:A:1243:GLU:O	1:A:1246:VAL:HG12	2.19	0.43
1:A:1549:THR:HG22	1:A:1554:ALA:HA	2.00	0.43
1:D:1384:ASN:HA	1:D:1387:ARG:HG3	2.01	0.43
1:D:1734:PHE:CE2	1:D:1751:LEU:HD13	2.53	0.43
1:D:1751:LEU:O	1:D:1782:ILE:HG22	2.18	0.43
1:D:1803:ILE:HD12	1:D:1831:LEU:HD21	2.00	0.43
1:D:2292:ILE:HD12	1:D:2293:LYS:N	2.34	0.43
1:E:726:TYR:O	1:E:737:THR:OG1	2.32	0.43
1:E:1405:LEU:HD22	1:E:1406:GLY:N	2.34	0.43
1:E:1931:PRO:HB2	1:E:1991:ARG:CG	2.49	0.43
1:C:1394:ILE:HB	1:C:1403:LEU:HD12	2.00	0.43
1:B:1004:GLY:O	1:B:1071:LYS:NZ	2.44	0.43
1:B:1186:THR:HG22	1:B:1186:THR:O	2.19	0.43
1:A:682:VAL:C	1:A:683:LEU:HD12	2.39	0.43
1:A:1014:ARG:O	1:A:1018:LYS:CA	2.57	0.43
1:D:1180:PHE:HB2	1:D:1234:GLY:N	2.33	0.43
1:D:1293:ILE:HG22	1:D:1294:LYS:N	2.34	0.43
1:D:2088:LEU:HD23	1:D:2093:TRP:HB2	2.00	0.43
1:D:2091:GLY:O	1:D:2095:VAL:HG22	2.18	0.43
1:E:1079:LEU:HD12	1:E:1444:ASN:HA	2.01	0.43
1:E:1832:VAL:HG21	1:E:1838:THR:HG23	2.01	0.43
1:E:2053:MET:HB2	1:F:1863:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1411:GLU:OE2	1:C:1412:VAL:HG12	2.18	0.43
1:F:1411:GLU:OE2	1:F:1412:VAL:HG12	2.19	0.43
1:F:1945:THR:O	1:F:1947:LYS:N	2.51	0.43
1:F:2088:LEU:O	1:F:2115:GLY:HA2	2.18	0.43
1:B:682:VAL:C	1:B:683:LEU:HD12	2.39	0.43
1:D:1067:THR:HG22	1:D:1082:ARG:N	2.34	0.42
1:E:1437:ALA:HB3	1:E:1481:VAL:HG23	1.99	0.42
1:E:1484:ASP:O	1:E:1488:ILE:HD12	2.17	0.42
1:C:2088:LEU:O	1:C:2115:GLY:HA2	2.19	0.42
1:B:662:PRO:HG2	1:B:665:THR:HG23	2.01	0.42
1:B:919:LYS:HA	1:B:922:MET:HG2	2.01	0.42
1:A:947:SER:O	1:A:950:ALA:HB3	2.19	0.42
1:A:1120:LEU:HD22	1:A:1155:ARG:HE	1.83	0.42
1:D:1426:ILE:CD1	1:D:1476:ASN:HD21	2.32	0.42
1:D:2135:LYS:HA	1:D:2138:ARG:HG2	2.01	0.42
1:E:896:LEU:HD12	1:E:899:LEU:HD11	2.01	0.42
1:E:986:VAL:HG23	1:E:987:VAL:N	2.34	0.42
1:E:1571:MET:SD	1:E:1575:THR:OG1	2.66	0.42
1:E:2113:SER:O	1:E:2114:ARG:NH1	2.47	0.42
1:E:2327:SER:HB2	1:E:2330:GLN:HG2	2.01	0.42
1:C:1680:ILE:HD13	1:C:1699:PHE:CD1	2.53	0.42
1:C:2026:THR:HG22	1:C:2030:ILE:CD1	2.49	0.42
1:F:1711:ILE:HG22	1:F:1905:SER:CB	2.49	0.42
1:F:1931:PRO:HB2	1:F:1991:ARG:HB3	2.00	0.42
1:F:2018:TRP:HZ3	1:F:2023:ALA:HA	1.84	0.42
1:B:933:LEU:HD12	1:B:933:LEU:O	2.18	0.42
1:B:1524:LYS:HD3	1:B:1526:ILE:HD11	2.01	0.42
1:D:930:THR:HG22	1:D:930:THR:O	2.20	0.42
1:D:1367:ASP:OD1	1:D:1368:ARG:N	2.53	0.42
1:D:1475:LEU:HD13	1:D:1475:LEU:C	2.39	0.42
1:E:1682:ASN:HD22	1:E:1719:ASN:ND2	2.16	0.42
1:E:2101:ASN:H	1:E:2105:MET:CE	2.31	0.42
1:A:689:SER:O	1:A:692:SER:N	2.48	0.42
1:A:1069:LEU:HD11	1:A:1078:ALA:CB	2.44	0.42
1:D:1703:SER:O	1:D:1706:ALA:HB3	2.20	0.42
1:D:2322:MET:HG2	1:C:2308:VAL:HG11	2.01	0.42
1:E:1766:SER:O	1:E:1787:GLY:N	2.48	0.42
1:C:1707:ARG:HD3	1:C:1810:ALA:HB2	2.02	0.42
1:F:1807:SER:O	1:F:1810:ALA:HB3	2.20	0.42
1:F:2041:MET:CE	1:F:2079:LEU:HD12	2.49	0.42
1:F:2119:GLU:OE1	1:F:2121:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1374:GLU:OE2	1:D:1376:ALA:HB3	2.20	0.42
1:D:1842:GLU:HG2	1:D:1872:ILE:HD13	2.02	0.42
1:D:2019:PHE:HB2	1:D:2021:ASP:OD1	2.19	0.42
1:E:1108:ILE:HG21	1:E:1144:VAL:HG12	2.01	0.42
1:E:1605:PHE:HE2	1:E:1679:VAL:HG21	1.83	0.42
1:E:1807:SER:HB2	1:E:1834:LEU:CD2	2.50	0.42
1:E:1819:LEU:HD23	1:E:1819:LEU:N	2.34	0.42
1:F:1761:VAL:HA	1:F:1764:LEU:HD12	2.01	0.42
1:F:2103:ARG:NH2	1:F:2229:LYS:HD2	2.34	0.42
1:B:1130:ILE:O	1:B:1130:ILE:HG22	2.19	0.42
1:A:1418:ASP:OD2	1:A:1420:ARG:NH1	2.49	0.42
1:A:1496:VAL:HG11	1:A:1540:LEU:HD12	2.02	0.42
1:D:2297:ARG:HE	1:C:2314:VAL:HG13	1.83	0.42
1:E:1031:HIS:O	1:E:1034:VAL:HG23	2.20	0.42
1:E:1988:VAL:HG12	1:E:2045:ASN:HD22	1.83	0.42
1:E:2182:VAL:HG22	1:F:1748:TYR:HE1	1.83	0.42
1:E:2325:HIS:O	1:E:2326:ILE:HD13	2.20	0.42
1:C:2224:LEU:HB2	1:C:2274:LEU:HD13	2.01	0.42
1:C:2291:ASN:C	1:C:2295:ILE:HD12	2.38	0.42
1:B:992:ARG:HE	1:B:1062:ILE:CD1	2.33	0.42
1:B:995:LEU:HD23	1:B:996:ARG:N	2.34	0.42
1:B:998:GLU:O	1:B:1002:GLN:HG2	2.19	0.42
1:B:1451:LEU:HD23	1:B:1502:ARG:HH12	1.83	0.42
1:A:869:LEU:HD12	1:A:1036:LYS:HD2	2.01	0.42
1:A:998:GLU:O	1:A:1002:GLN:HG2	2.19	0.42
1:D:988:MET:O	1:D:991:LEU:HG	2.19	0.42
1:D:1528:ILE:HG22	1:D:1528:ILE:O	2.19	0.42
1:E:935:GLN:N	1:E:935:GLN:OE1	2.52	0.42
1:C:1517:ILE:CD1	1:C:1528:ILE:HD13	2.49	0.42
1:C:2122:GLY:O	1:C:2125:GLU:HG2	2.20	0.42
1:C:2135:LYS:HA	1:C:2138:ARG:CD	2.50	0.42
1:B:851:ARG:O	1:B:855:TYR:HB3	2.19	0.42
1:D:869:LEU:HD12	1:D:1036:LYS:HD2	2.01	0.42
1:D:874:PHE:CZ	1:D:878:VAL:HG11	2.54	0.42
1:D:1510:GLN:NE2	1:D:1512:GLU:HG3	2.34	0.42
1:D:1977:ARG:HD3	1:D:1980:GLY:HA2	2.02	0.42
1:D:2251:TRP:HA	1:D:2254:GLU:HG2	2.01	0.42
1:E:1253:MET:HB2	1:E:1321:ASP:OD2	2.19	0.42
1:C:1727:ALA:O	1:C:1730:ILE:HG22	2.20	0.42
1:F:1421:PHE:CE2	1:F:1468:THR:HG21	2.55	0.42
1:F:1827:ILE:O	1:F:1831:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2067:ILE:HG23	1:F:2068:VAL:N	2.35	0.42
1:A:1511:ALA:HB3	1:A:1532:LEU:HB2	2.01	0.42
1:D:933:LEU:HD12	1:D:933:LEU:O	2.20	0.42
1:D:1031:HIS:O	1:D:1034:VAL:HG23	2.19	0.42
1:D:1055:LEU:HD11	1:D:1060:LEU:HD22	2.02	0.42
1:D:1079:LEU:HD23	1:D:1079:LEU:HA	1.78	0.42
1:D:2119:GLU:OE2	1:D:2122:GLY:N	2.53	0.42
1:C:2082:ILE:HD12	1:C:2082:ILE:N	2.35	0.42
1:F:1705:LEU:C	1:F:1705:LEU:HD13	2.40	0.42
1:F:2016:GLN:HE21	1:F:2045:ASN:HD21	1.68	0.42
1:B:1316:LYS:O	1:B:1319:LEU:N	2.52	0.42
1:A:1246:VAL:HG23	1:A:1311:PHE:CE1	2.55	0.42
1:D:683:LEU:HD21	1:D:697:MET:SD	2.60	0.42
1:D:1078:ALA:O	1:D:1081:ALA:HB3	2.19	0.42
1:D:1682:ASN:OD1	1:D:1683:ASP:N	2.53	0.42
1:D:1934:PRO:HD3	1:D:1989:GLU:HA	2.02	0.42
1:E:638:HIS:CD2	1:E:736:ILE:HG23	2.55	0.42
1:E:856:VAL:HG11	1:E:885:LEU:HB2	2.02	0.42
1:E:992:ARG:CZ	1:E:995:LEU:HD13	2.50	0.42
1:E:1384:ASN:HA	1:E:1387:ARG:HB2	2.01	0.42
1:E:1421:PHE:CD2	1:E:1457:LEU:HD21	2.55	0.42
1:C:1761:VAL:HA	1:C:1764:LEU:HD12	2.01	0.42
1:D:1076:LYS:CD	1:D:1077:VAL:HG23	2.48	0.41
1:D:1421:PHE:CE1	1:D:1460:ALA:HB1	2.55	0.41
1:E:1293:ILE:HG22	1:E:1294:LYS:N	2.34	0.41
1:E:2119:GLU:OE2	1:E:2122:GLY:N	2.53	0.41
1:C:1812:ASN:HA	1:C:2035:ARG:NH1	2.34	0.41
1:F:1492:VAL:O	1:F:1496:VAL:HG12	2.20	0.41
1:F:2030:ILE:HG23	1:F:2040:LEU:CD1	2.49	0.41
1:A:849:LEU:HB3	1:A:897:LEU:HD22	2.02	0.41
1:D:694:VAL:HG11	1:D:870:PRO:HG3	2.01	0.41
1:D:962:PHE:O	1:D:966:GLN:HB2	2.19	0.41
1:D:1774:ASP:HB3	1:D:1779:ARG:HD2	2.02	0.41
1:E:1589:GLN:O	1:E:1593:LEU:HD13	2.19	0.41
1:C:2118:LEU:HD12	1:C:2119:GLU:HG3	2.02	0.41
1:B:850:HIS:H	1:B:897:LEU:HD23	1.85	0.41
1:B:1135:PRO:HA	1:B:1138:PHE:CD1	2.55	0.41
1:A:655:LEU:HD11	1:A:1021:MET:H	1.85	0.41
1:A:1104:PHE:CE2	1:A:1133:VAL:HG23	2.55	0.41
1:D:1147:MET:HE1	1:D:1168:HIS:HB3	2.03	0.41
1:D:1483:MET:H	1:D:1517:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1981:ILE:HD12	1:D:1983:VAL:CG1	2.50	0.41
1:E:682:VAL:HG11	1:E:698:ASN:HB3	2.02	0.41
1:E:1599:TYR:OH	1:E:1650:ARG:NH2	2.53	0.41
1:C:1382:GLU:OE2	1:C:1424:ARG:NH1	2.42	0.41
1:C:1555:GLN:HB3	1:C:1572:LEU:HD21	2.02	0.41
1:B:963:MET:HG3	1:B:966:GLN:HE21	1.85	0.41
1:B:1052:ASP:HA	1:B:1055:LEU:HD21	2.02	0.41
1:A:726:TYR:HB2	1:A:737:THR:OG1	2.20	0.41
1:A:731:VAL:HG13	1:A:732:ASP:N	2.36	0.41
1:D:915:GLU:O	1:D:919:LYS:HG2	2.20	0.41
1:D:1865:SER:O	1:D:1868:GLN:HB2	2.20	0.41
1:E:933:LEU:HD12	1:E:933:LEU:O	2.20	0.41
1:E:1632:LEU:HD12	1:E:1632:LEU:O	2.20	0.41
1:A:1066:LEU:CD2	1:A:1081:ALA:HB2	2.51	0.41
1:E:878:VAL:O	1:E:882:VAL:HG23	2.20	0.41
1:E:1133:VAL:O	1:E:1136:ASN:N	2.52	0.41
1:E:1180:PHE:HB2	1:E:1234:GLY:N	2.35	0.41
1:E:1598:ILE:HG13	1:E:1599:TYR:H	1.86	0.41
1:E:1865:SER:O	1:E:1868:GLN:HB2	2.21	0.41
1:E:2068:VAL:O	1:E:2071:LEU:HD23	2.21	0.41
1:C:1511:ALA:HB3	1:C:1532:LEU:HB2	2.02	0.41
1:B:1034:VAL:O	1:B:1038:ASN:N	2.53	0.41
1:B:1496:VAL:HG11	1:B:1540:LEU:HD12	2.02	0.41
1:B:1535:GLU:N	1:B:1535:GLU:OE1	2.54	0.41
1:A:639:VAL:HG21	1:A:734:TYR:CZ	2.55	0.41
1:D:1154:VAL:HG22	1:D:1180:PHE:HE1	1.86	0.41
1:D:1489:GLU:OE2	1:D:1493:ARG:NH2	2.54	0.41
1:D:1534:ASN:HD22	1:D:1535:GLU:N	2.18	0.41
1:D:1817:ILE:HG22	1:D:1818:SER:N	2.36	0.41
1:E:1421:PHE:CZ	1:E:1460:ALA:HB1	2.55	0.41
1:C:1558:PHE:CZ	1:C:1573:ILE:HD13	2.55	0.41
1:C:1919:ILE:HA	1:C:2212:ARG:HE	1.86	0.41
1:F:1439:PHE:CE1	1:F:1481:VAL:HG21	2.56	0.41
1:B:849:LEU:HB3	1:B:897:LEU:HD22	2.02	0.41
1:A:990:LEU:O	1:A:993:GLN:HB3	2.21	0.41
1:A:1524:LYS:CD	1:A:1526:ILE:HD11	2.50	0.41
1:D:1829:ALA:CB	1:D:1846:LEU:HD11	2.51	0.41
1:F:1410:VAL:HG12	1:F:1411:GLU:N	2.36	0.41
1:F:1539:TYR:CE1	1:F:1629:SER:HA	2.55	0.41
1:A:1154:VAL:CG2	1:A:1178:VAL:HG11	2.51	0.41
1:D:1104:PHE:O	1:D:1108:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1253:MET:HB2	1:D:1321:ASP:OD2	2.21	0.41
1:E:628:THR:O	1:E:632:VAL:HG23	2.21	0.41
1:E:1405:LEU:HD22	1:E:1406:GLY:H	1.86	0.41
1:E:1429:HIS:O	1:E:1430:SER:HB3	2.20	0.41
1:E:2097:ASP:HA	1:E:2107:MET:HE1	2.01	0.41
1:C:1733:MET:HG3	1:C:1753:LEU:CD1	2.51	0.41
1:F:1534:ASN:HD22	1:F:1535:GLU:N	2.18	0.41
1:F:1834:LEU:HD13	1:F:1834:LEU:O	2.20	0.41
1:B:1013:LEU:HD13	1:B:1024:VAL:HG13	2.02	0.41
1:B:1060:LEU:O	1:B:1060:LEU:HD13	2.20	0.41
1:A:1040:LEU:HD23	1:A:1040:LEU:O	2.21	0.41
1:A:1473:ILE:HB	1:A:1511:ALA:HA	2.02	0.41
1:D:1105:LEU:HD21	1:D:1137:PHE:CE2	2.55	0.41
1:D:1421:PHE:HB2	1:D:1471:ASN:OD1	2.20	0.41
1:D:1766:SER:CB	1:D:1788:LYS:HD3	2.51	0.41
1:D:1809:LEU:O	1:D:1812:ASN:N	2.54	0.41
1:D:2059:GLN:NE2	1:C:1878:ASN:O	2.54	0.41
1:D:2173:GLU:HA	1:D:2176:ILE:HD12	2.02	0.41
1:E:1534:ASN:ND2	1:E:1537:GLY:O	2.53	0.41
1:E:1688:ILE:HG22	1:E:1688:ILE:O	2.20	0.41
1:E:1846:LEU:HD23	1:E:1875:MET:HG3	2.03	0.41
1:E:1880:VAL:HG13	1:F:2061:LEU:HD11	2.02	0.41
1:C:1385:ARG:HG3	1:C:1575:THR:O	2.21	0.41
1:C:1995:LEU:C	1:C:1995:LEU:HD13	2.41	0.41
1:C:2243:GLN:HE21	1:B:947:SER:HB2	1.86	0.41
1:F:1483:MET:HG3	1:F:1484:ASP:H	1.85	0.41
1:F:1597:TYR:O	1:F:1601:ILE:HD12	2.21	0.41
1:F:1925:PHE:CD2	1:F:1937:MET:HA	2.55	0.41
1:F:2244:ILE:O	1:F:2248:LEU:HD23	2.21	0.41
1:B:952:LEU:HD23	1:B:961:PHE:CG	2.56	0.41
1:B:1129:SER:HB2	1:B:1428:ARG:HE	1.86	0.41
1:B:1154:VAL:HG22	1:B:1180:PHE:HE1	1.86	0.41
1:B:1246:VAL:HG13	1:B:1247:ARG:NH1	2.36	0.41
1:A:848:LYS:O	1:A:852:VAL:HG23	2.20	0.41
1:A:992:ARG:HE	1:A:1062:ILE:CD1	2.34	0.41
1:A:1060:LEU:HD13	1:A:1060:LEU:O	2.21	0.41
1:A:1079:LEU:HD21	1:A:1448:ARG:N	2.36	0.41
1:A:1129:SER:CB	1:A:1428:ARG:HE	2.34	0.41
1:A:1390:ASP:HB2	1:A:1409:LYS:HB3	2.02	0.41
1:A:1428:ARG:HB3	1:A:1478:VAL:HG23	2.02	0.41
1:D:2053:MET:HB2	1:C:1863:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2108:TYR:OH	1:E:2218:ARG:NH2	2.49	0.41
1:C:1699:PHE:O	1:C:1703:SER:OG	2.27	0.41
1:F:1995:LEU:HD13	1:F:1995:LEU:C	2.42	0.41
1:F:2082:ILE:HD12	1:F:2082:ILE:N	2.36	0.41
1:B:655:LEU:HD13	1:B:1021:MET:HB3	2.03	0.41
1:D:960:VAL:HG12	1:D:964:ASN:HD21	1.84	0.40
1:D:1165:SER:HB2	1:D:1181:GLN:HG3	2.04	0.40
1:D:1767:VAL:HG12	1:D:1785:ILE:HA	2.03	0.40
1:D:2068:VAL:O	1:D:2071:LEU:HD23	2.20	0.40
1:D:2322:MET:HE1	1:C:2315:ALA:HA	2.03	0.40
1:E:979:ILE:HD12	1:E:980:ARG:HB2	2.03	0.40
1:E:1070:SER:O	1:E:1071:LYS:HE2	2.21	0.40
1:E:1782:ILE:HG23	1:E:1782:ILE:O	2.21	0.40
1:E:1943:HIS:NE2	1:E:1945:THR:OG1	2.53	0.40
1:E:2096:ILE:HD12	1:E:2096:ILE:O	2.20	0.40
1:C:1503:LEU:O	1:C:1507:ARG:N	2.54	0.40
1:C:2041:MET:SD	1:C:2079:LEU:HD12	2.61	0.40
1:C:2144:TYR:CZ	1:C:2168:LEU:HD11	2.57	0.40
1:F:1568:LEU:HD21	1:F:1571:MET:HB2	2.02	0.40
1:F:1991:ARG:NH1	1:F:1993:VAL:HA	2.36	0.40
1:B:990:LEU:HD23	1:B:993:GLN:OE1	2.20	0.40
1:B:1028:ILE:HA	1:B:1031:HIS:HD2	1.87	0.40
1:A:1080:ARG:HA	1:A:1083:GLN:HG2	2.03	0.40
1:D:874:PHE:O	1:D:877:LYS:N	2.54	0.40
1:E:919:LYS:HA	1:E:922:MET:HG2	2.02	0.40
1:E:1120:LEU:CD1	1:E:1152:VAL:HG23	2.51	0.40
1:E:1598:ILE:HG21	1:E:1683:ASP:HB3	2.03	0.40
1:E:2117:VAL:HG23	1:F:1797:LEU:HD21	2.03	0.40
1:C:2000:ASP:H	1:C:2006:SER:HG	1.63	0.40
1:F:1437:ALA:O	1:F:1441:TYR:HB2	2.21	0.40
1:A:1014:ARG:HA	1:A:1021:MET:HE2	2.03	0.40
1:D:1598:ILE:HD12	1:D:1660:VAL:HG21	2.03	0.40
1:E:1137:PHE:HB3	1:E:1145:VAL:HG11	2.03	0.40
1:E:1305:ALA:HA	1:E:1308:PHE:HB2	2.03	0.40
1:E:1596:THR:OG1	1:E:1888:ASP:OD2	2.27	0.40
1:E:1995:LEU:O	1:E:2011:ILE:N	2.46	0.40
1:C:1507:ARG:HH11	1:C:1507:ARG:HG3	1.85	0.40
1:C:1662:TRP:HB2	1:C:1664:MET:SD	2.61	0.40
1:C:2224:LEU:CB	1:C:2274:LEU:HD13	2.51	0.40
1:F:2082:ILE:HD12	1:F:2082:ILE:H	1.86	0.40
1:B:640:ALA:CB	1:B:685:VAL:HG11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:848:LYS:O	1:D:852:VAL:HG23	2.21	0.40
1:D:988:MET:HE1	1:D:1059:LEU:HA	2.04	0.40
1:D:1457:LEU:HD22	1:D:1457:LEU:N	2.37	0.40
1:E:1945:THR:O	1:E:1947:LYS:N	2.54	0.40
1:C:1509:LEU:HD12	1:C:1534:ASN:O	2.22	0.40
1:F:1978:LEU:HD11	1:F:2212:ARG:HG3	2.04	0.40
1:B:889:LEU:HD23	1:B:889:LEU:O	2.21	0.40
1:B:1572:LEU:HD12	1:B:1572:LEU:N	2.37	0.40
1:D:726:TYR:O	1:D:737:THR:OG1	2.30	0.40
1:D:1289:LEU:CD2	1:D:1291:VAL:HG13	2.51	0.40
1:D:1301:ASP:HA	1:D:1304:LEU:HD12	2.04	0.40
1:D:1585:SER:O	1:D:1589:GLN:NE2	2.55	0.40
1:D:1965:GLN:HG3	1:D:1966:PRO:HD3	2.04	0.40
1:D:2280:GLU:OE1	1:D:2285:HIS:NE2	2.54	0.40
1:D:2328:PRO:HA	1:D:2331:ARG:HG3	2.02	0.40
1:C:1410:VAL:HG12	1:C:1411:GLU:N	2.36	0.40
1:C:1539:TYR:CE1	1:C:1629:SER:HA	2.56	0.40
1:F:1660:VAL:HG22	1:F:1661:ALA:N	2.37	0.40
1:F:2026:THR:HG22	1:F:2030:ILE:CD1	2.50	0.40
1:F:2144:TYR:CZ	1:F:2168:LEU:HD11	2.56	0.40
1:B:971:LEU:HA	1:B:974:ARG:HE	1.87	0.40
1:B:1329:PHE:HB2	1:B:1356:PHE:HB2	2.03	0.40
1:B:1373:LEU:CD1	1:B:1378:ALA:HB2	2.51	0.40
1:A:668:ASN:ND2	1:A:868:CYS:SG	2.95	0.40
1:A:1024:VAL:O	1:A:1027:TYR:HB2	2.21	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	741/2407 (31%)	640 (86%)	93 (13%)	8 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	741/2407 (31%)	641 (86%)	93 (13%)	7 (1%)	17	56
1	C	940/2407 (39%)	882 (94%)	51 (5%)	7 (1%)	22	62
1	D	1498/2407 (62%)	1367 (91%)	123 (8%)	8 (0%)	29	68
1	E	1498/2407 (62%)	1371 (92%)	117 (8%)	10 (1%)	22	62
1	F	940/2407 (39%)	883 (94%)	51 (5%)	6 (1%)	25	65
All	All	6358/14442 (44%)	5784 (91%)	528 (8%)	46 (1%)	26	62

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	868	CYS
1	D	1304	LEU
1	E	868	CYS
1	E	1304	LEU
1	C	2326	ILE
1	F	2326	ILE
1	B	868	CYS
1	B	1304	LEU
1	A	868	CYS
1	A	1304	LEU
1	D	1580	LYS
1	C	1580	LYS
1	C	2276	LYS
1	F	2276	LYS
1	B	873	PHE
1	B	1055	LEU
1	A	873	PHE
1	D	873	PHE
1	E	1580	LYS
1	C	2325	HIS
1	F	1580	LYS
1	F	2325	HIS
1	B	1360	ALA
1	A	1093	TYR
1	A	1360	ALA
1	D	1400	LYS
1	E	873	PHE
1	E	1400	LYS
1	C	2327	SER
1	F	2327	SER

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Mol	Chain	Res	Type
1	A	1053	PRO
1	D	1360	ALA
1	E	994	TYR
1	E	1172	LYS
1	E	1688	ILE
1	A	1138	PHE
1	D	1146	ARG
1	E	1759	LYS
1	C	1400	LYS
1	B	1053	PRO
1	B	1428	ARG
1	A	1400	LYS
1	D	1688	ILE
1	E	1548	VAL
1	F	1688	ILE
1	C	1688	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	694/2108 (33%)	675 (97%)	19 (3%)	44	66
1	B	694/2108 (33%)	678 (98%)	16 (2%)	50	70
1	C	830/2108 (39%)	807 (97%)	23 (3%)	43	65
1	D	1354/2108 (64%)	1321 (98%)	33 (2%)	49	69
1	E	1354/2108 (64%)	1310 (97%)	44 (3%)	39	62
1	F	830/2108 (39%)	817 (98%)	13 (2%)	62	79
All	All	5756/12648 (46%)	5608 (97%)	148 (3%)	49	67

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	875	SER
1	D	889	LEU

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Mol	Chain	Res	Type
1	D	909	ARG
1	D	947	SER
1	D	974	ARG
1	D	995	LEU
1	D	996	ARG
1	D	1022	ASN
1	D	1076	LYS
1	D	1079	LEU
1	D	1095	LEU
1	D	1175	THR
1	D	1236	MET
1	D	1373	LEU
1	D	1381	LEU
1	D	1388	ASN
1	D	1403	LEU
1	D	1438	SER
1	D	1449	LEU
1	D	1470	CYS
1	D	1480	THR
1	D	1502	ARG
1	D	1534	ASN
1	D	1649	ASN
1	D	1797	LEU
1	D	1914	ASN
1	D	1915	SER
1	D	2003	ASN
1	D	2116	SER
1	D	2161	ARG
1	D	2245	GLN
1	D	2286	SER
1	D	2327	SER
1	E	644	LEU
1	E	674	LEU
1	E	734	TYR
1	E	860	LEU
1	E	864	MET
1	E	875	SER
1	E	889	LEU
1	E	909	ARG
1	E	947	SER
1	E	974	ARG
1	E	983	MET

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Mol	Chain	Res	Type
1	E	990	LEU
1	E	1022	ASN
1	E	1061	ASN
1	E	1080	ARG
1	E	1085	LEU
1	E	1095	LEU
1	E	1098	ASN
1	E	1125	LEU
1	E	1232	ARG
1	E	1381	LEU
1	E	1388	ASN
1	E	1391	LEU
1	E	1438	SER
1	E	1449	LEU
1	E	1451	LEU
1	E	1480	THR
1	E	1518	ARG
1	E	1528	ILE
1	E	1534	ASN
1	E	1540	LEU
1	E	1571	MET
1	E	1649	ASN
1	E	1758	TYR
1	E	1914	ASN
1	E	2003	ASN
1	E	2025	LYS
1	E	2034	ASN
1	E	2111	ARG
1	E	2116	SER
1	E	2135	LYS
1	E	2161	ARG
1	E	2245	GLN
1	E	2327	SER
1	C	1381	LEU
1	C	1384	ASN
1	C	1438	SER
1	C	1467	ARG
1	C	1478	VAL
1	C	1498	ARG
1	C	1518	ARG
1	C	1534	ASN
1	C	1540	LEU

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Mol	Chain	Res	Type
1	C	1541	ASP
1	C	1564	LYS
1	C	1622	LEU
1	C	1649	ASN
1	C	1806	GLU
1	C	1843	ASN
1	C	1902	MET
1	C	2003	ASN
1	C	2116	SER
1	C	2138	ARG
1	C	2168	LEU
1	C	2181	GLN
1	C	2240	THR
1	C	2327	SER
1	F	1381	LEU
1	F	1438	SER
1	F	1467	ARG
1	F	1478	VAL
1	F	1518	ARG
1	F	1534	ASN
1	F	1540	LEU
1	F	1649	ASN
1	F	1843	ASN
1	F	2003	ASN
1	F	2116	SER
1	F	2240	THR
1	F	2327	SER
1	B	897	LEU
1	B	916	LYS
1	B	974	ARG
1	B	1080	ARG
1	B	1233	MET
1	B	1250	ASP
1	B	1253	MET
1	B	1325	ARG
1	B	1377	LEU
1	B	1381	LEU
1	B	1487	LYS
1	B	1514	LYS
1	B	1518	ARG
1	B	1534	ASN
1	B	1540	LEU

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Mol	Chain	Res	Type
1	B	1564	LYS
1	A	637	LEU
1	A	734	TYR
1	A	897	LEU
1	A	916	LYS
1	A	920	LYS
1	A	947	SER
1	A	974	ARG
1	A	1034	VAL
1	A	1105	LEU
1	A	1175	THR
1	A	1303	ARG
1	A	1377	LEU
1	A	1381	LEU
1	A	1398	ASN
1	A	1438	SER
1	A	1502	ARG
1	A	1518	ARG
1	A	1534	ASN
1	A	1540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	638	HIS
1	D	653	HIS
1	D	668	ASN
1	D	859	ASN
1	D	862	ASN
1	D	964	ASN
1	D	1000	GLN
1	D	1022	ASN
1	D	1026	ASN
1	D	1114	GLN
1	D	1140	HIS
1	D	1314	GLN
1	D	1315	ASN
1	D	1384	ASN
1	D	1388	ASN
1	D	1402	HIS
1	D	1429	HIS
1	D	1443	GLN

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Mol	Chain	Res	Type
1	D	1444	ASN
1	D	1565	GLN
1	D	1589	GLN
1	D	1655	ASN
1	D	1796	ASN
1	D	1840	GLN
1	D	1914	ASN
1	D	2003	ASN
1	D	2045	ASN
1	D	2059	GLN
1	D	2146	HIS
1	E	653	HIS
1	E	859	ASN
1	E	862	ASN
1	E	940	GLN
1	E	964	ASN
1	E	993	GLN
1	E	1005	HIS
1	E	1022	ASN
1	E	1033	GLN
1	E	1061	ASN
1	E	1083	GLN
1	E	1099	GLN
1	E	1114	GLN
1	E	1181	GLN
1	E	1388	ASN
1	E	1443	GLN
1	E	1444	ASN
1	E	1510	GLN
1	E	1589	GLN
1	E	1649	ASN
1	E	1655	ASN
1	E	1682	ASN
1	E	1914	ASN
1	E	1969	GLN
1	E	2003	ASN
1	E	2085	GLN
1	E	2146	HIS
1	E	2243	GLN
1	E	2321	HIS
1	C	1534	ASN
1	C	1619	GLN

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Mol	Chain	Res	Type
1	C	1649	ASN
1	C	1965	GLN
1	C	2003	ASN
1	C	2013	GLN
1	C	2016	GLN
1	C	2076	GLN
1	C	2181	GLN
1	C	2234	ASN
1	F	1534	ASN
1	F	1565	GLN
1	F	1649	ASN
1	F	1796	ASN
1	F	1836	GLN
1	F	2003	ASN
1	F	2013	GLN
1	F	2028	GLN
1	F	2045	ASN
1	F	2076	GLN
1	F	2181	GLN
1	F	2243	GLN
1	F	2277	GLN
1	B	668	ASN
1	B	940	GLN
1	B	966	GLN
1	B	1005	HIS
1	B	1026	ASN
1	B	1083	GLN
1	B	1181	GLN
1	B	1315	ASN
1	B	1534	ASN
1	A	939	GLN
1	A	940	GLN
1	A	966	GLN
1	A	973	GLN
1	A	982	HIS
1	A	1005	HIS
1	A	1026	ASN
1	A	1181	GLN
1	A	1315	ASN
1	A	1333	GLN
1	A	1472	HIS
1	A	1534	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

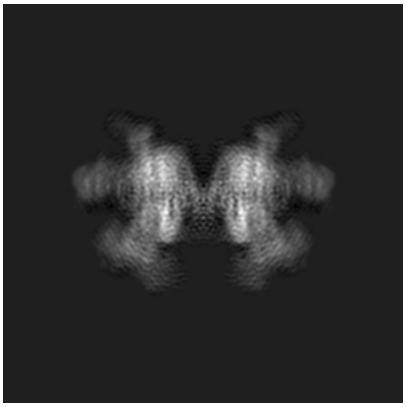
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4343. These allow visual inspection of the internal detail of the map and identification of artifacts.

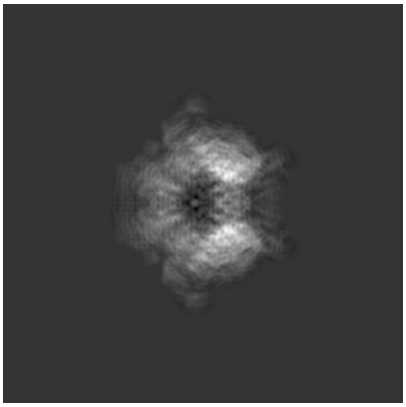
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

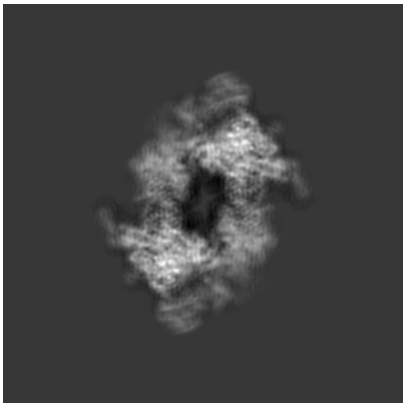
6.1.1 Primary map



X



Y

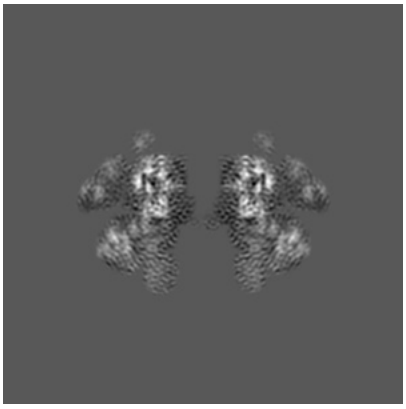


Z

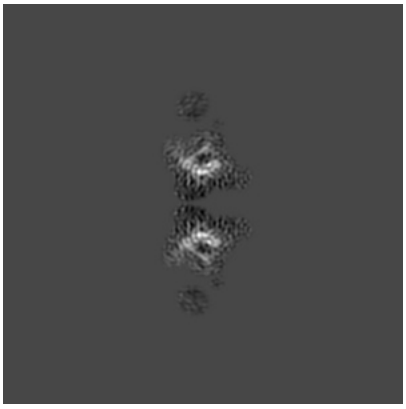
The images above show the map projected in three orthogonal directions.

6.2 Central slices

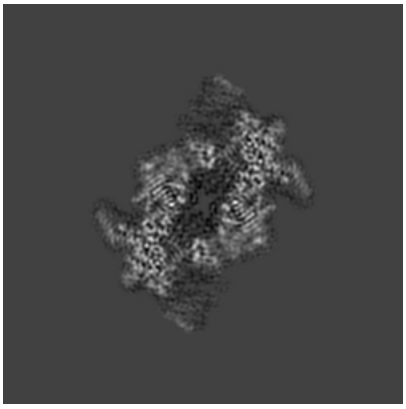
6.2.1 Primary map



X Index: 188



Y Index: 188

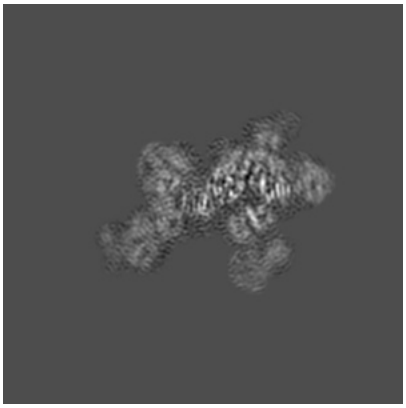


Z Index: 188

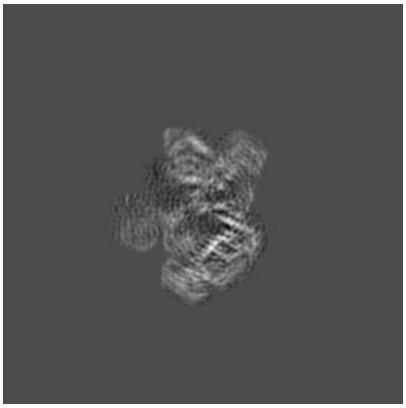
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

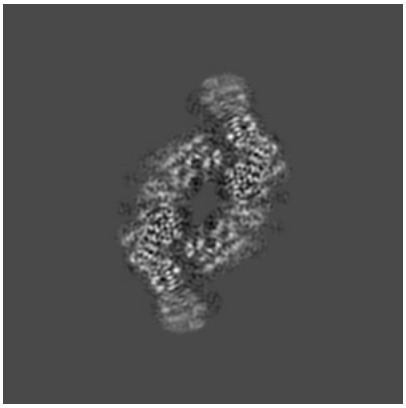
6.3.1 Primary map



X Index: 219



Y Index: 153



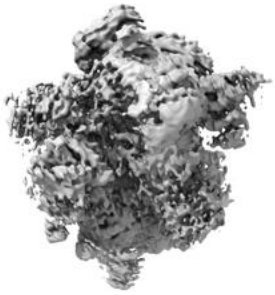
Z Index: 201

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

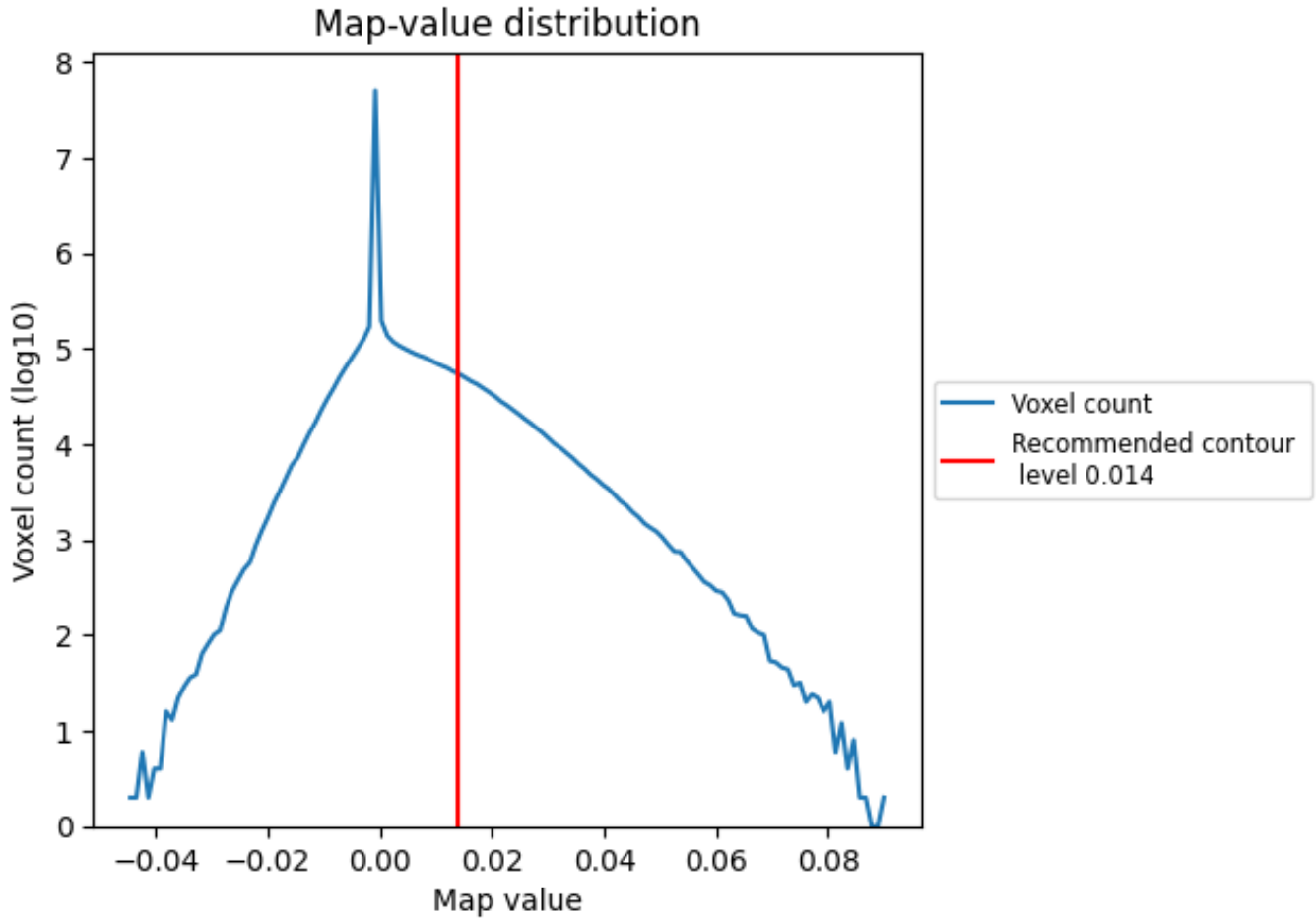
6.5 Mask visualisation (i)

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

7 Map analysis

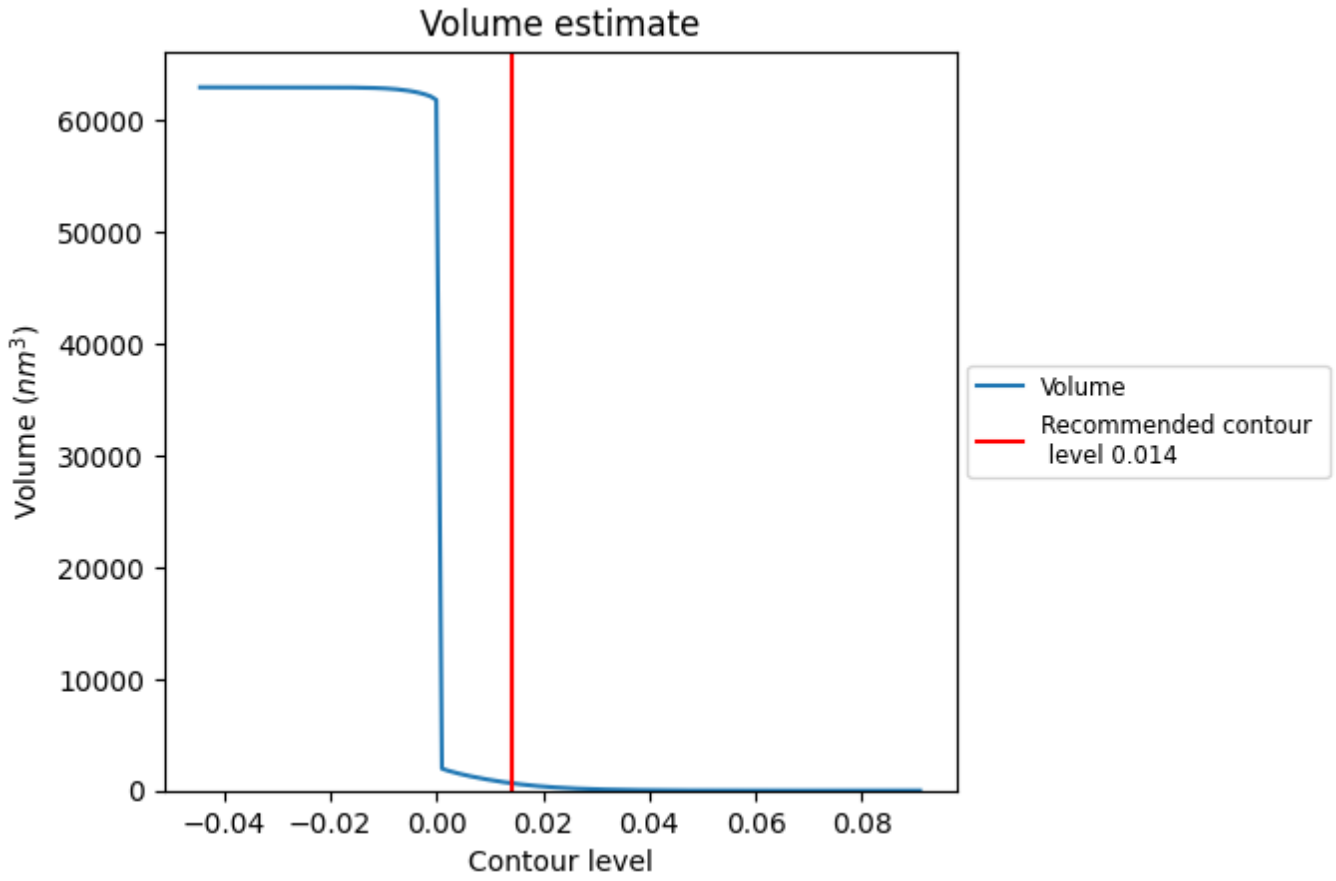
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

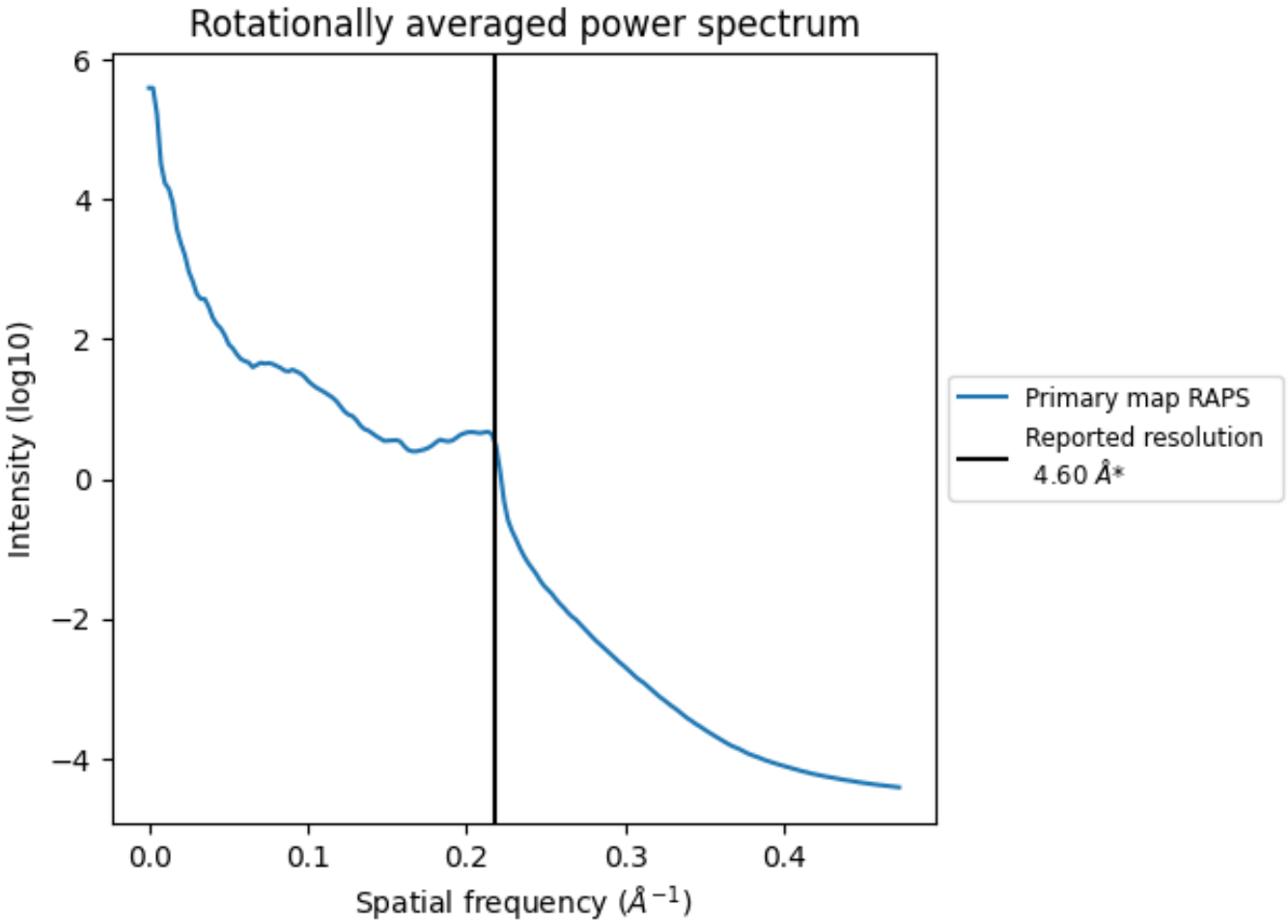
7.2 Volume estimate



The volume at the recommended contour level is 664 nm^3; this corresponds to an approximate mass of 600 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 0.217 Å^{-1}

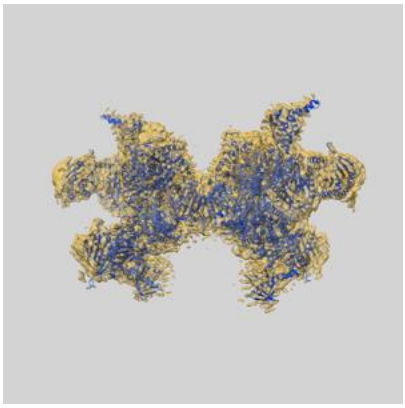
8 Fourier-Shell correlation (i)

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

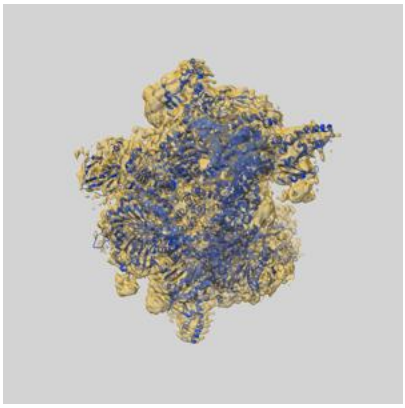
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4343 and PDB model 6G2H. Per-residue inclusion information can be found in section 3 on page 13.

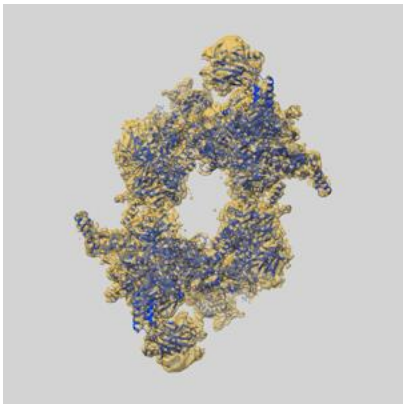
9.1 Map-model overlay



X



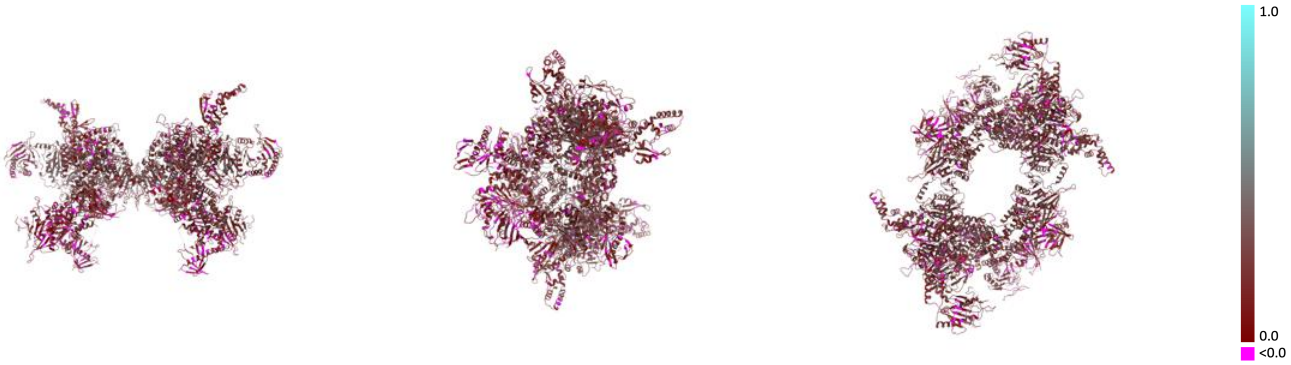
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

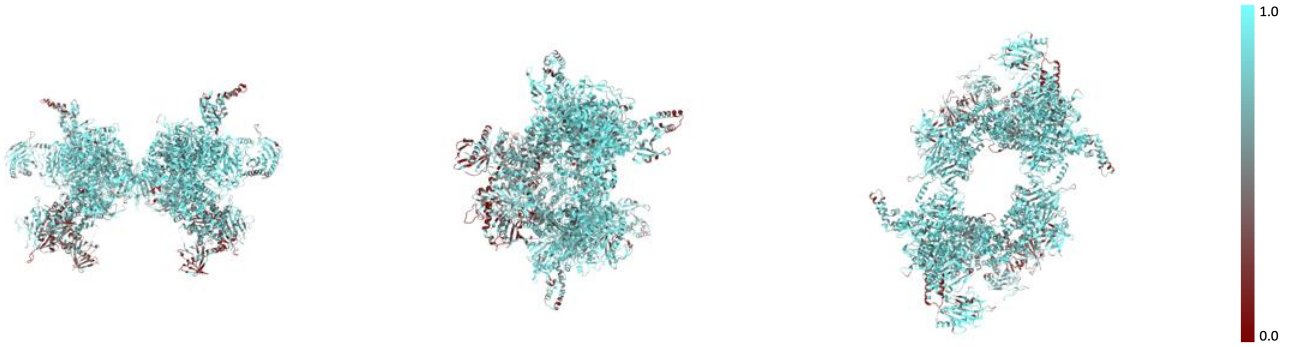
9.2 Q-score mapped to coordinate model



X Y Z

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.

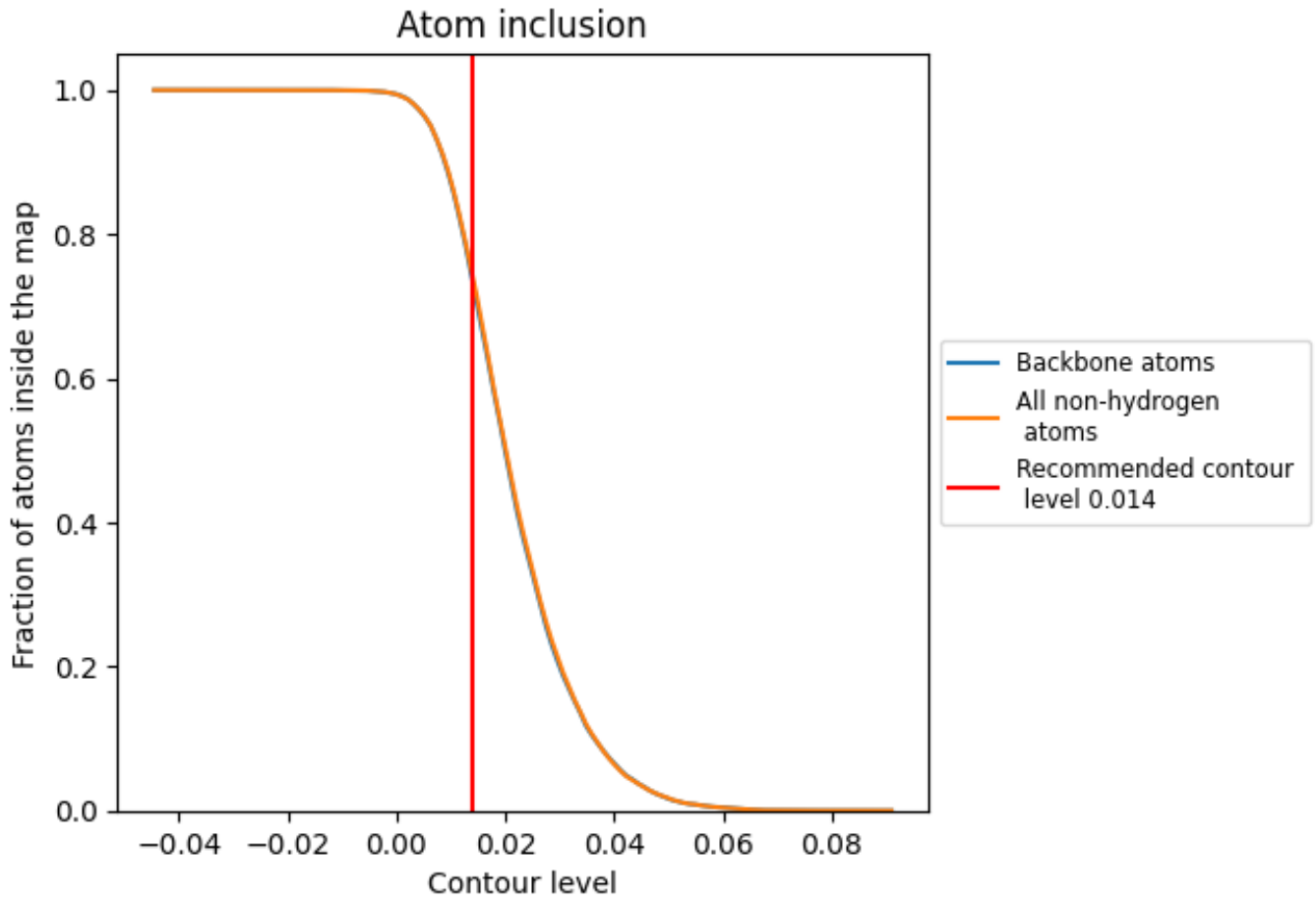
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7407	0.2070
A	0.5563	0.1510
B	0.5518	0.1490
C	0.8001	0.2210
D	0.8040	0.2250
E	0.8041	0.2280
F	0.7989	0.2210