



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:59 PM UTC

PDB ID : 6G2H / pdb_00006g2h
EMDB ID : EMD-4343
Title : Filament of acetyl-CoA carboxylase and BRCT domains of BRCA1 (ACC-BRCT) core at 4.6 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stüttfeld, 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:

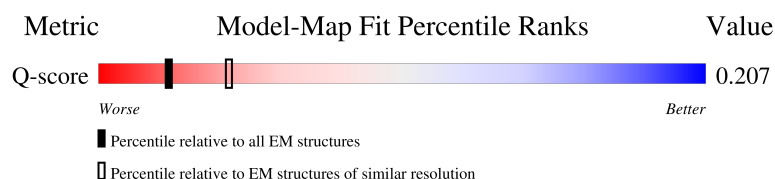
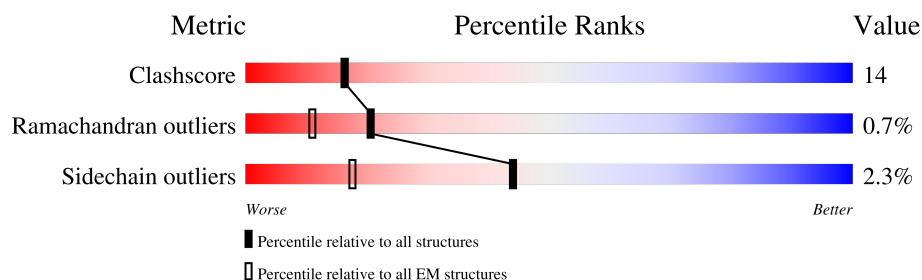
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

Mol	Chain	Length	Quality of chain
1	A	2407	
1	B	2407	
1	C	2407	
1	D	2407	

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Mol	Chain	Length	Quality of chain
1	E	2407	42% 20% 37%
1	F	2407	28% 11% 61%

2 Entry composition

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

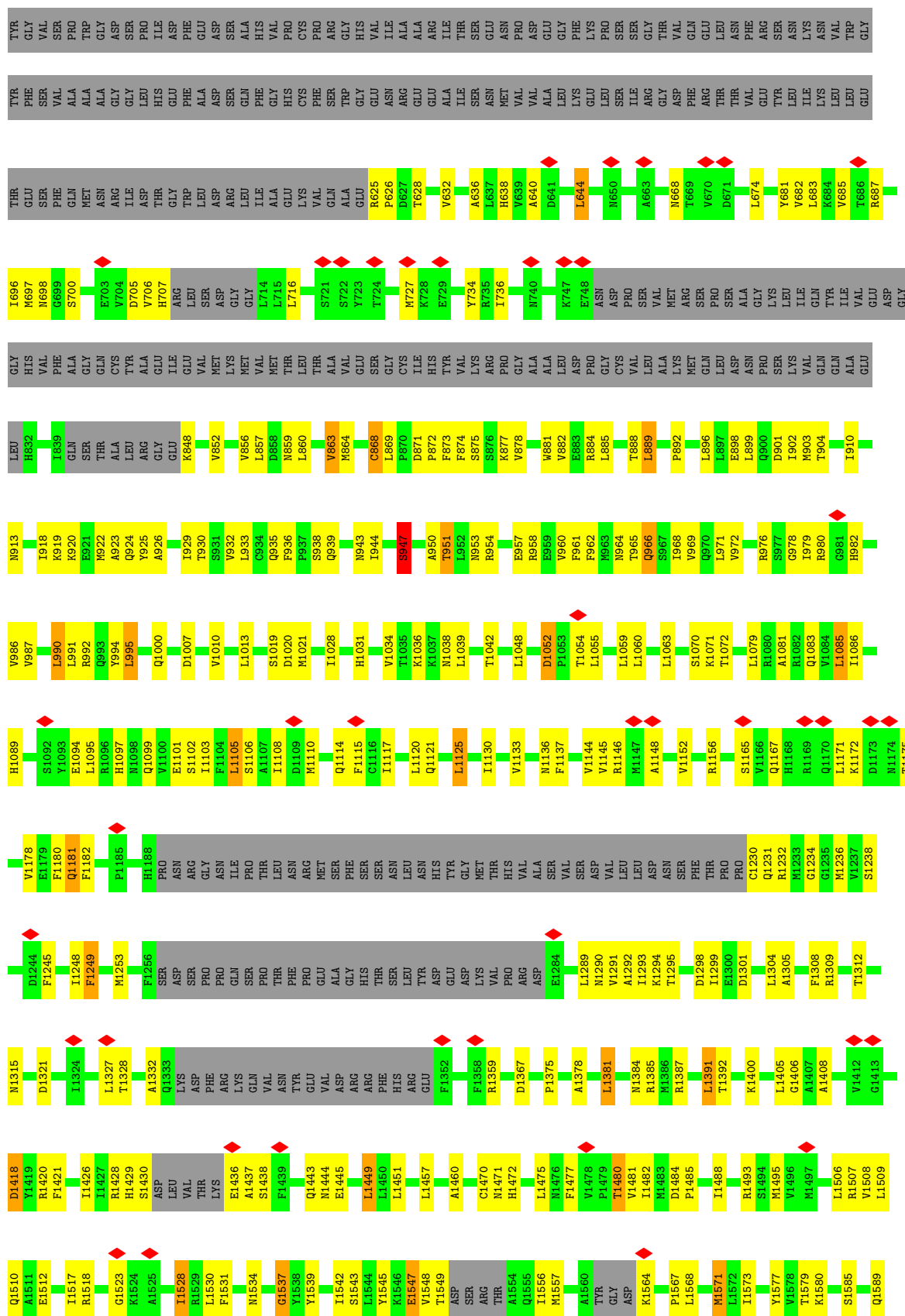
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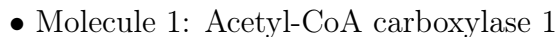
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	LYS	-	expression tag	UNP Q13085
A	-10	LYS	-	expression tag	UNP Q13085
A	-9	ALA	-	expression tag	UNP Q13085
A	-8	GLY	-	expression tag	UNP Q13085
A	-7	LEU	-	expression tag	UNP Q13085
A	-6	GLU	-	expression 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

Y925	Y994	L1079	R1169	G1235	T1312	K1400	T1480	N1682	TYR	H1768	A1779	E1695	M1571	L1782	I1783	D1784	L1698	F1699	I1786	G1787	K1788	L1797	R1798	I1803	A1804	G1805	S1808	L1809	M1812	E1813	I1814	L1817	S1818	F1734	H1735	V1736	T1821	A1824	A1829	Y1830	L1831	V1832	L1837	T1838	E1842	H1845	L1846	T1849	H1864	S1865
A926	L995	R1081	Q1170	M1236	N1315	H1401	M1483	I1684	GLY	C1769	R1779	D1696	M1571	I1782	T1783	D1784	L1698	F1699	I1786	G1787	K1788	L1797	R1798	I1803	A1804	G1805	S1808	L1809	M1812	E1813	I1814	L1817	S1818	F1734	H1735	V1736	T1821	A1824	A1829	Y1830	L1831	V1832	L1837	T1838	E1842	H1845	L1846	T1849	H1864	S1865



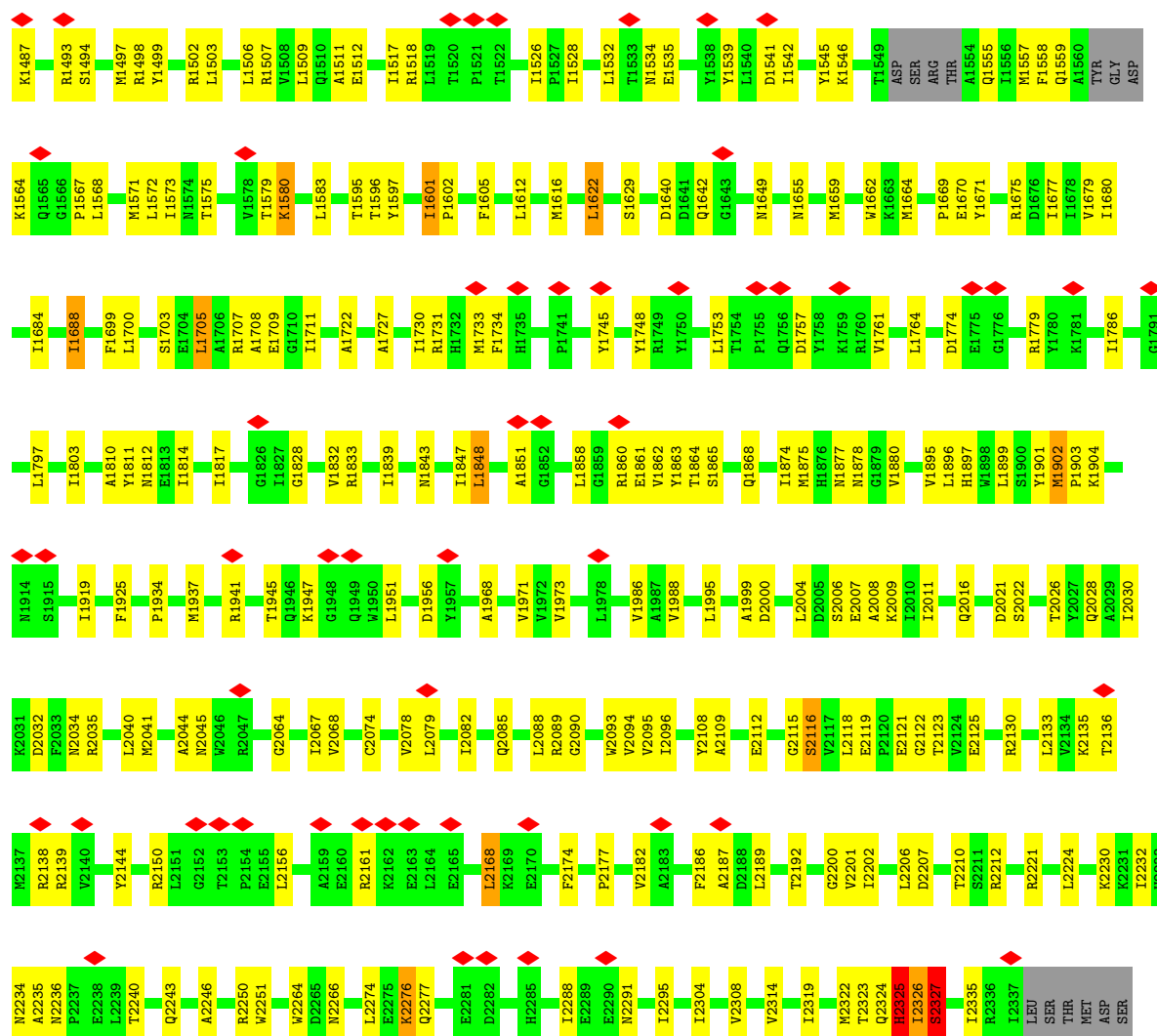




Frequency	Percentage
Daily	28%
Weekly	11%
Monthly	61%









- Molecule 1: Acetyl-CoA carboxylase 1

[illegible]





[illegible]

- Molecule 1: Acetyl-CoA carboxylase 1

[illegible]

GLY	MET	ASP	GLU	PRO	SER	PRO	LEU	ALA	GLN	PRO	GLU	LEU	ASN	GLN	HIS	SER	ARG	PHE	ILE	ILE	GLY	SER	VAL	SER	GLU	ASP	ASN	SER	GLU	ASN	LEU	VAL	LYS	LYS	GLU	GLY	SER	LEU	PRO	ALA	SER	VAL	GLY	ASP	THR	LEU
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SER	ASP	LEU	GLY	ILE	SER	SER	LEU	GLN	ASP	GLY	LEU	ALA	LEU	HIS	ILE	ARG	SER	SER	NET	SER	SER	GLY	LEU	HIS	LEU	VAL	LYS	GLN	GLY	ARG	ASP	ARG	ARG	ASP	LYS	LYS	ILE	ASP	SER	ASP	GLN	ARG	ARG	ASP	PHE	THR	THR	VAL	GLU	PHE	VAL	THR	ARG	PHE	GLY	GLY	ASN	LYS	VAL	ILE	THR
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LYS VAL LEU LEU ILE ILE ASN ASN GLY ILE ILE ALA ALA ALA ALA VAL VAL LYS CYS MET MET ARG ARG SER SER ILE ILE ARG ARG TRP TRP SER SER TYR TYR GLU GLU MET MET PHE PHE ARG ARG ASN ASN GLU GLU ARG ARG ALA ALA ILE ILE ARG ARG PHE PHE VAL VAL VAL VAL ASP ASP LEU LEU LYS LYS ALA ALA ASN ASN ALA ALA GLU GLU TYR TYR ILE ILE LYS LYS MET MET MET MET ASP ASP HIS HIS TYR TYR VAL VAL PRO PRO VAL VAL PRO PRO

GLY	GLY	PRO	PRO	ASN	ASN	ASN	TYR	ASN	ASN	ALA	ALA	VAL	ASP	LEU	ILE	ALA	LYS	ARG	ALA	ILE	PRO	VAL	GLN	ALA	VAL	TRP	TRP	GLY	HIS	ALA	SER	GLY	ASN	PRO	LYS	LEU	PRO	GLY	GLY
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LEU GLY ASP ASP LYS ILE ALA SER SER ILE VAL ALA ALA GLN THR GLY ALA GLY ILE PRO THR LEU PRO TRP TRP SER SER GLY SER GLY LEU ARG ARG ASP ASP TRP TRP GLN GLU GLU ASN ASP PHE SER LYS ARG ILE LEU LEU TYR TYR GLU LYS GLY TYR VAL VAL ASP VAL PRO GLN GLU TYR TYR VAL VAL ASP ASP ASP ASP LEU LEU THR THR

ALA ALA ALA GLU VAL GLY TYR PRO PRO MET MET ILE ILE LYS ALA ALA SER GLU GLY GLY GLY GLY LYS VAL VAL ASN ASN ALA ALA ASP ASP PHE PHE PRO PRO ASN ASN LEU LEU PHE PHE ARG ARG GLN GLN VAL VAL GLN GLN ALA GLU VAL VAL PRO PRO GLY GLY SER SER PRO PRO ILE ILE PHE PHE VAL VAL MET MET ARG ARG LEU LEU ALA ALA LYS LYS GLN GLN SER SER HIS HIS LEU LEU THR THR

VAL	GLN	ILE	LEU	ALA	ASP	GLN	TYR	GLY	ASN	ILE	ALA	ILE	SER	LEU	PHE	GLY	ARG	ASP	CYS	SER	VAL	GLN	GLN	ARG	ARG	HIS	LYS	ILE	ILE	GLU	GLU	ALA	ALA	ALA	ALA	ALA	VAL	PHE	GLU	HIS	HIS	MET	GLU	MET	GLN	CYS	ALA	VAL	VAL	VAL	GLY	TYR	VAL	SER
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[illegible]

Tyr	Gly	Val	Ser	Pro	Trp	Gly	Asp	Ser	Pro	Pro	Ile	Asp	Phe	Glu	Asp	Ser	Ala	His	Val	Pro	Cys	Pro	Arg	Gly	His	Val	Ile	Ala	Ala	Arg	Ile	Thr	Ser	Glu	Pro	Pro	Asp	Gly	Gly	Phe	Lys	Pro	Ser	Ser	Gly	Thr	Val	Gln	Glu	Leu	Asn	Asn	Phe	Arg	Ser	Asn	Lys	Val	Ala	Val	Trp	Tyr
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Tyr	Phe	Ser	Val	Ala	Ala	Gly	Leu	His	Glu	Phe	Ala	Asn	Ser	Gln	Phe	Gly	His	Cys	Phe	Ser	Trp	Ser	Gly	Glu	Asn	Arg	Glu	Glu	Ala	Ile	Ser	Met	Val	Val	Ala	Ala	Leu	Lys	Glu	Leu	Ser	Ile	Arg	Gly	ASP	Phe	Arg	Thr	Thr	Val	Val	Glu	Tyr	Leu	Ile	Lys	Leu	Leu
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THR	GLU	SER	PRO	GLN	MET	ASN	ARG	ILE	ASP	THR	GLY	TRP	LEU	ASP	ARG	LEU	ILE	ALA	GLU	LYS	VAL	GLN	ALA	ALA	GLU	R625	R626	D627	T628	M629	L630	G631	V632	V633	V634	G635	A636	L637	H638	V639	A640	D641	L644	R645	G646	S647	V648	S649	N650	H653	S654	L655	E656	R657	G658	A663	H664
T685	L666	L667	M668	T669	V670	D671	V672	E673	L674	L675	V676	E677	G678	V679	V680	V681	V682	L683	R684	V685	T686	R687	G688	S689	G692	V693	V694	V695	L696	M697	V702	D705	V706	H707	ARG	LEU	SER	ASP	GLY	GLY	L714	S717	V718	D719	G720	S721	S722	V723	T724	T725	V726	M727	K728	E729	T730		

V731	D732	R733	Y734	R735	I736	T737	I738	G739	N740	K741	T742	E746	K747	E748	ASP	ASN	PRO	SER	VAL	MET	ARG	SER	PRO	SER	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	TYR
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ALA	VAL	GLU	SER	GLY	CYS	ILE	HIS	TYR	VAL	LYS	ARG	PRO	GLY	ALA	ALA	LEU	ASP	ASN	PRO	SER	PRO	LYS	VAL	VAL	GLN	GLN	ALA	ALA	LEU	LEU	H832	H833	G834	S835	L836	R837	R838	I839	GLN	SER	THR	ALA	ALA	LEU	LEU	ARG	GLY	GLU	K848	L849	H850	R851	V852
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CYS	ASN	PHE	ARG	LYS	GLU	PRO	ILE	ILE	ILE
ILE	ALA	ILE	GLY	ASP	LEU	LEU	ARG	TRP	MET
SER	ASN	ILE	SER	MET	SER	THR	TRP	ASN	HIS
ARG	PRO	ILE	VAL	TYR	TYR	ILE	MET	ASN	ASN
ASP	GLU	PRO	LEU	ASP	LEU	GLN	PRO	LEU	GLY
TYR	LEU	TYR	GLU	GLN	VAL	ALA	ALA	ALA	LEU
VAL	THR	HIS	PRO	VAL	ASP	VAL	GLY	GLY	VAL
LEU	ASP	GLN	GLU	LEU	PRO	GLU	ARG	THR	THR
LYS	GLY	VAL	GLY	PHE	LYS	ALA	PRO	HIS	CYS
GLN	GLN	ALA	THR	PHE	ASN	CYS	HIS	CYS	ARG
ILE	ILE	VAL	VAL	GLY	LEU	GLY	PRO	THR	ALA
ARG	GLN	GLN	GLU	ALA	ASP	LEU	THR	VAL	ILE
SER	ALA	PHE	ILE	TYR	SER	ARG	GLN	CYS	GLY
LEU	MET	ALA	LYS	ILE	GLY	VAL	LYS	ASP	ILE
VAL	LEU	ASP	PHE	VAL	ASP	PHE	GLY	ASP	GLY
VAL	LEU	GLN	THR	GLY	ARG	VAL	GLN	PHE	ALA
ALA	ARG	HIS	ARG	GLY	ILE	TRP	LEU	GLY	LEU
ASN	TRP	ASP	LYS	LEU	ILE	LEU	LEU	GLY	THR
PRO	PRO	THR	ASP	ARG	GLN	GLN	SER	VAL	VAL
GLU	VAL	PRO	LEU	GLU	GLU	GLN	GLN	PHE	ARG
VAL	VAL	GLY	VAL	CYS	GLY	ALA	PHE	THR	LEU
ALA	VAL	ARG	LYS	CYS	GLY	ALA	PHE	VAL	GLY
MET	GLU	MET	THR	GLN	GLN	GLN	ASP	LEU	GLN
GLY	GLY	GLN	MET	PRO	VAL	VAL	TYR	HIS	ARG
ASP	THR	GLN	GLU	VAL	VAL	GLY	GLY	THR	THR
SER	THR	SER	GLY	VAL	THR	THR	GLY	THR	ARG
ILE	VAL	LYS	LYS	VAL	PHE	ARG	SER	LEU	ILE
ILE	VAL	GLY	GLY	VAL	VAL	VAL	SER	LEU	GLN
HIS	ALA	VAL	VAL	TYR	ILE	ILE	THR	HIS	ILE
MET	THR	ILE	SER	PRO	THR	ASP	GLU	LEU	LEU
THR	VAL	SER	SER	ASN	LYS	LYS	THR	SER	THR
GLN	TRP	ASP	THR	ASN	GLU	GLN	ALA	ALA	GLY
HIS	ASN	ASP	ASP	ASN	LEU	LEU	GLY	GLY	GLY
ILE	LEU	LYS	GLY	VAL	THR	THR	VAL	VAL	LEU
ARG	GLU	PHE	PRO	VAL	ASN	ARG	GLY	ASN	ASN
ILE	GLU	ILE	GLU	VAL	VAL	VAL	GLY	LEU	LEU
ARG	LYS	TYR	GLU	ILE	ARG	ILE	ALA	SER	LYS
ILE	GLN	TRP	SER	ASP	THR	SER	VAL	VAL	VAL
LEU	LEU	ARG	THR	SER	LEU	THR	LEU	PRO	THR
SER	THR	LEU	ALA	SER	ALA	ALA	GLY	GLY	GLY
THR	GLU	ARG	GLU	ILE	PHE	THR	VAL	ASP	ASN
MET	GLU	ARG	GLU	ASN	ARG	GLU	ILE	ARG	VAL
ASP	GLU	LEU	ARG	PRO	VAL	VAL	PRO	ILE	THR
SER	GLY	LEU	GLU	PRO	PHE	VAL	VAL	ILE	TYR
PRO	VAL	LEU	LEU	HIS	LEU	GLY	GLY	GLY	THR
SER	HIS	GLU	GLU	MET	GLU	GLU	VAL	PHE	SER
THR	VAL	LEU	LEU	GLU	ASP	THR	VAL	VAL	ASN
					MET	TYR	ALA	VAL	ASN
					THR	VAL	GLN	PRO	ASN
					ARG	VAL	THR	THR	GLN
					GLY	ALA	VAL	THR	LEU
					ASP	GLY	THR	THR	GLY
					GLU	ARG	ARG	PRO	GLY
					GLU	GLY	GLY	VAL	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
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					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
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					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
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					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
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					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
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					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	GLY
					GLU	GLY	GLY	THR	

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	1.21	25/8496 (0.3%)
1	B	0.52	0/6291	1.18	24/8496 (0.3%)
1	C	0.63	0/7780	1.07	14/10540 (0.1%)
1	D	0.66	2/12491 (0.0%)	1.21	60/16905 (0.4%)
1	E	0.65	1/12491 (0.0%)	1.15	30/16905 (0.2%)
1	F	0.63	1/7780 (0.0%)	1.07	17/10540 (0.2%)
All	All	0.62	4/53124 (0.0%)	1.15	170/71882 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1601	ILE	CA-CB	-9.81	1.49	1.54
1	E	1625	PRO	CA-C	-9.24	1.46	1.51
1	F	1625	PRO	CA-C	-7.18	1.48	1.51
1	D	1625	PRO	CA-C	-5.97	1.48	1.51

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1545	TYR	CA-C-N	10.74	139.60	122.21
1	D	1545	TYR	C-N-CA	10.74	139.60	122.21
1	A	1052	ASP	CA-C-N	10.71	133.23	119.84
1	A	1052	ASP	C-N-CA	10.71	133.23	119.84
1	D	1500	GLY	CA-C-N	8.23	131.31	120.28
1	D	1500	GLY	C-N-CA	8.23	131.31	120.28
1	D	1648	MET	CA-C-N	8.20	133.97	122.41
1	D	1648	MET	C-N-CA	8.20	133.97	122.41
1	E	1072	THR	N-CA-C	7.93	120.63	111.11
1	F	1546	LYS	N-CA-C	-7.67	97.65	109.24
1	C	1546	LYS	N-CA-C	-7.65	97.68	109.24
1	F	1731	ARG	CB-CA-C	-7.33	98.22	110.68
1	E	1485	PRO	N-CA-C	7.20	127.30	112.47
1	D	1503	LEU	CA-CB-CG	7.19	141.47	116.30
1	F	1441	TYR	CA-CB-CG	6.96	126.43	113.90
1	D	1441	TYR	CA-CB-CG	6.87	126.26	113.90
1	E	2336	ARG	CB-CG-CD	6.84	127.04	111.30
1	A	1075	ALA	N-CA-C	-6.80	105.61	114.04
1	D	1461	PHE	CA-C-N	6.77	129.24	120.44
1	D	1461	PHE	C-N-CA	6.77	129.24	120.44
1	D	1459	VAL	CA-C-N	6.73	129.30	120.28
1	D	1459	VAL	C-N-CA	6.73	129.30	120.28
1	D	1533	THR	N-CA-C	6.68	119.92	108.02
1	D	2035	ARG	CB-CG-CD	6.65	126.58	111.30
1	E	1428	ARG	CB-CA-C	6.61	121.81	111.77
1	A	1053	PRO	N-CA-C	6.57	126.00	112.47
1	A	1426	ILE	N-CA-C	-6.56	98.18	108.81
1	D	1072	THR	N-CA-C	6.54	118.96	111.11
1	D	2035	ARG	CG-CD-NE	-6.46	97.79	112.00
1	A	1381	LEU	CA-CB-CG	6.46	138.91	116.30
1	C	2327	SER	N-CA-C	6.30	123.72	109.81
1	F	2327	SER	N-CA-C	6.29	123.71	109.81
1	E	1625	PRO	O-C-N	-6.29	118.42	121.31
1	B	1375	PRO	N-CA-C	6.27	121.99	113.84
1	B	1516	ASN	N-CA-C	-6.22	99.87	109.76
1	D	995	LEU	N-CA-C	-6.18	103.86	111.40
1	B	1175	THR	N-CA-C	6.14	118.90	108.90
1	B	1028	ILE	CA-C-N	6.13	128.49	120.28
1	B	1028	ILE	C-N-CA	6.13	128.49	120.28
1	C	2325	HIS	CA-C-N	6.10	132.95	121.97
1	C	2325	HIS	C-N-CA	6.10	132.95	121.97
1	E	1537	GLY	N-CA-C	-6.08	105.02	112.68
1	D	1373	LEU	CA-C-N	6.06	132.31	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1373	LEU	C-N-CA	6.06	132.31	121.76
1	D	1038	ASN	N-CA-C	-6.00	104.07	111.40
1	D	1438	SER	N-CA-C	5.96	117.45	111.07
1	D	2096	ILE	N-CA-C	5.91	121.63	109.34
1	D	1485	PRO	N-CA-C	5.90	124.62	112.47
1	D	1393	ALA	CA-C-N	5.88	128.45	123.04
1	D	1393	ALA	C-N-CA	5.88	128.45	123.04
1	A	1137	PHE	N-CA-C	5.88	120.52	113.23
1	E	995	LEU	N-CA-C	-5.87	104.24	111.40
1	A	1104	PHE	CB-CA-C	-5.82	102.00	110.96
1	D	2059	GLN	N-CA-C	5.81	123.18	110.80
1	E	1902	MET	N-CA-C	5.78	118.87	110.14
1	F	2325	HIS	CA-C-N	5.77	132.35	121.97
1	F	2325	HIS	C-N-CA	5.77	132.35	121.97
1	A	1375	PRO	N-CA-C	5.76	121.33	113.84
1	D	1053	PRO	N-CA-C	5.75	124.32	112.47
1	A	1539	TYR	N-CA-C	-5.75	101.33	109.96
1	D	1156	ARG	CG-CD-NE	5.75	124.64	112.00
1	D	1632	LEU	N-CA-C	5.75	118.58	108.75
1	B	1368	ARG	CB-CG-CD	5.74	124.50	111.30
1	E	1156	ARG	CG-CD-NE	5.73	124.61	112.00
1	E	1579	THR	CA-C-N	5.70	132.43	121.54
1	E	1579	THR	C-N-CA	5.70	132.43	121.54
1	A	1132	ASP	N-CA-C	5.69	118.58	111.24
1	D	1422	PHE	N-CA-CB	5.68	119.89	110.52
1	E	2221	ARG	CG-CD-NE	-5.65	99.56	112.00
1	E	2059	GLN	N-CA-C	5.64	122.82	110.80
1	D	1537	GLY	N-CA-C	-5.64	105.58	112.68
1	A	1093	TYR	CB-CA-C	5.61	121.58	110.42
1	D	867	TYR	CA-C-N	5.59	132.22	121.54
1	D	867	TYR	C-N-CA	5.59	132.22	121.54
1	D	1477	PHE	N-CA-CB	5.58	118.88	109.94
1	D	1662	TRP	CA-CB-CG	5.57	124.19	113.60
1	D	1079	LEU	CA-CB-CG	-5.56	96.86	116.30
1	C	2200	GLY	N-CA-C	5.56	123.64	115.08
1	D	1428	ARG	CA-CB-CG	5.55	125.20	114.10
1	B	1381	LEU	CA-CB-CG	5.55	135.72	116.30
1	B	1243	GLU	N-CA-C	-5.54	105.16	111.14
1	B	1137	PHE	N-CA-C	5.54	119.75	112.89
1	A	645	ARG	CA-CB-CG	-5.53	103.04	114.10
1	B	884	ARG	CB-CA-C	-5.52	101.62	110.79
1	B	884	ARG	CA-CB-CG	5.51	125.11	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1368	ARG	CB-CG-CD	5.50	123.94	111.30
1	E	1758	TYR	CA-CB-CG	5.48	123.77	113.90
1	B	1093	TYR	CB-CA-C	5.48	121.33	110.42
1	B	645	ARG	CA-CB-CG	-5.48	103.15	114.10
1	E	889	LEU	N-CA-C	-5.46	106.46	113.23
1	A	1028	ILE	CA-C-N	5.45	127.58	120.28
1	A	1028	ILE	C-N-CA	5.45	127.58	120.28
1	A	1239	PHE	CA-C-N	5.45	133.57	121.80
1	A	1239	PHE	C-N-CA	5.45	133.57	121.80
1	E	2127	LYS	CD-CE-NZ	5.43	129.27	111.90
1	D	1712	PRO	N-CA-C	5.39	119.95	111.38
1	B	1176	CYS	N-CA-C	-5.39	99.95	108.73
1	D	1418	ASP	CA-C-N	5.37	131.80	121.54
1	D	1418	ASP	C-N-CA	5.37	131.80	121.54
1	F	1625	PRO	O-C-N	-5.37	118.84	121.31
1	F	2138	ARG	CB-CG-CD	5.37	123.64	111.30
1	D	1579	THR	CA-C-N	5.36	131.78	121.54
1	D	1579	THR	C-N-CA	5.36	131.78	121.54
1	A	645	ARG	CB-CA-C	5.36	119.69	110.79
1	D	1670	GLU	N-CA-CB	-5.35	102.06	110.30
1	C	1579	THR	CA-C-N	5.33	131.72	121.54
1	C	1579	THR	C-N-CA	5.33	131.72	121.54
1	A	1146	ARG	CB-CG-CD	5.31	123.50	111.30
1	B	1239	PHE	N-CA-C	5.30	117.88	109.50
1	E	1038	ASN	N-CA-C	-5.29	104.94	111.40
1	A	947	SER	CA-C-N	-5.28	112.23	122.06
1	A	947	SER	C-N-CA	-5.28	112.23	122.06
1	D	1426	ILE	CG1-CB-CG2	5.27	126.52	110.70
1	B	947	SER	CA-C-N	-5.27	112.26	122.06
1	B	947	SER	C-N-CA	-5.27	112.26	122.06
1	A	697	MET	N-CA-C	-5.27	99.19	108.20
1	F	2200	GLY	N-CA-C	5.27	123.19	115.08
1	E	1418	ASP	CA-C-N	5.27	129.11	121.26
1	E	1418	ASP	C-N-CA	5.27	129.11	121.26
1	D	1474	PHE	N-CA-C	5.26	116.99	108.41
1	B	697	MET	N-CA-C	-5.25	99.23	108.20
1	B	961	PHE	N-CA-C	-5.23	105.66	111.36
1	B	1029	PHE	N-CA-CB	-5.23	102.43	110.12
1	B	1539	TYR	N-CA-C	-5.23	102.11	109.96
1	E	966	GLN	N-CA-C	-5.23	106.58	113.12
1	B	637	LEU	CD1-CG-CD2	-5.22	99.32	110.80
1	E	2061	LEU	CA-CB-CG	5.22	134.56	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2221	ARG	CB-CA-C	-5.21	99.75	110.38
1	F	2220	ARG	CB-CG-CD	-5.20	99.34	111.30
1	D	1437	ALA	CA-C-N	5.19	127.19	120.44
1	D	1437	ALA	C-N-CA	5.19	127.19	120.44
1	D	1019	SER	N-CA-C	5.18	116.93	111.28
1	D	1059	LEU	N-CA-C	-5.18	105.08	111.40
1	E	947	SER	CA-C-N	-5.18	112.42	122.06
1	E	947	SER	C-N-CA	-5.18	112.42	122.06
1	D	947	SER	CA-C-N	-5.17	112.44	122.06
1	D	947	SER	C-N-CA	-5.17	112.44	122.06
1	C	2177	PRO	N-CA-C	5.17	123.12	112.47
1	E	1731	ARG	CB-CA-C	-5.17	101.90	110.68
1	A	995	LEU	N-CA-C	-5.16	105.10	111.40
1	F	1662	TRP	CA-CB-CG	5.16	123.39	113.60
1	C	2324	GLN	CA-C-N	5.15	131.38	121.54
1	C	2324	GLN	C-N-CA	5.15	131.38	121.54
1	F	1833	ARG	N-CA-C	-5.15	105.75	111.36
1	D	1902	MET	N-CA-C	5.14	117.97	110.10
1	E	1019	SER	N-CA-C	5.14	116.88	111.28
1	B	645	ARG	CB-CA-C	5.13	119.31	110.79
1	E	1723	ARG	CG-CD-NE	5.13	123.28	112.00
1	E	2096	ILE	N-CA-C	5.13	120.01	109.34
1	D	2192	THR	N-CA-C	5.12	118.08	110.39
1	C	1485	PRO	N-CA-C	5.12	123.01	112.47
1	D	1501	SER	CA-C-N	5.10	127.37	120.38
1	D	1501	SER	C-N-CA	5.10	127.37	120.38
1	D	966	GLN	N-CA-C	-5.10	106.75	113.12
1	F	2063	PHE	N-CA-C	-5.08	106.58	112.89
1	B	1146	ARG	CB-CG-CD	5.08	122.99	111.30
1	F	1579	THR	CA-C-N	5.08	131.25	121.54
1	F	1579	THR	C-N-CA	5.08	131.25	121.54
1	D	974	ARG	CA-C-N	5.08	129.51	121.44
1	D	974	ARG	C-N-CA	5.08	129.51	121.44
1	F	1485	PRO	N-CA-C	5.07	122.92	112.47
1	D	1384	ASN	N-CA-C	-5.07	107.09	113.28
1	C	1441	TYR	CA-CB-CG	5.05	122.99	113.90
1	A	1052	ASP	N-CA-C	5.05	120.96	109.81
1	E	1181	GLN	CA-C-N	-5.04	113.46	122.32
1	E	1181	GLN	C-N-CA	-5.04	113.46	122.32
1	F	2326	ILE	N-CA-C	5.03	119.80	109.34
1	C	2326	ILE	N-CA-C	5.02	119.79	109.34
1	C	1428	ARG	CB-CA-C	5.02	119.27	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1449	LEU	CB-CG-CD1	5.00	125.70	110.70

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
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

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Mol	Chain	Res	Type	Group
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

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	193	0
1	B	6177	6184	6209	180	0
1	C	7610	7561	7585	211	0
1	D	12235	12181	12225	388	0
1	E	12235	12181	12225	368	0
1	F	7610	7561	7585	218	0
All	All	52044	51852	52038	1476	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 (1476) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:864:MET:HE2	1:B:1040:LEU:HD22	1.54	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:864:MET:HE2	1:A:1040:LEU:HD22	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1039:LEU:O	1:B:1042:THR:OG1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1099:GLN:O	1:E:1102:SER:OG	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1172:LYS:NZ	1:A:1251:GLU:OE1	2.31	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: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:B:903:MET:HB2	1:B:922:MET:HE1	1.82	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:B:1386:MET:HE2	1:B:1391:LEU:HD23	1.81	0.62
1:D:1236:MET:HE2	1:D:1290:ASN:HB2	1.80	0.62
1:E:958:ARG:O	1:E:962:PHE:N	2.31	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:PRO:O	1:D:925:TYR:OH	2.11	0.61
1:E:2101:ASN:HB3	1:E:2105:MET:HE2	1.81	0.61
1:F:1504:TRP:CG	1:F:1538:TYR:HH	2.18	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:E:2100:ILE:HB	1:E:2105:MET:HE1	1.81	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:D:1235:GLY:C	1:D:1236:MET:HE3	2.26	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:1039:LEU:O	1:E:1042:THR:OG1	2.15	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: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
1:D:1680:ILE:HG21	1:D:1699:PHE:HD1	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:F:1570:GLY:O	1:F:1571:MET:HE2	2.03	0.59
1:D:883:GLU:HA	1:D:886:MET:HE2	1.85	0.58
1:C:1901:TYR:HB2	1:C:1902:MET:HE1	1.85	0.58
1:E:1518:ARG:NH1	1:E:1523:GLY:O	2.36	0.58
1:A:903:MET:HB2	1:A:922:MET:HE1	1.84	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:988:MET:HE1	1:D:1058:GLU:OE1	2.04	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:F:1874:ILE:HG22	1:F:1875:MET:HE2	1.86	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:B:705:ASP:OD1	1:B:717:SER:OG	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1874:ILE:HG22	1:C:1875:MET:HE2	1.87	0.57
1:B:1408:ALA:HB2	1:B:1418:ASP:HB2	1.87	0.57
1:D:1309:ARG:O	1:D:1312:THR:OG1	2.21	0.56
1:D:1748:TYR:CE1	1:C:2182:VAL:HG22	2.40	0.56
1:C:1664:MET:HE1	1:C:1679:VAL:CG1	2.35	0.56
1:E:1682:ASN:HD21	1:E:1718:ALA:C	2.12	0.56
1:E:1886:CYS:N	1:E:1890:GLU:OE2	2.34	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:A:929:ILE:O	1:A:930:THR:OG1	2.19	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:1684:ILE:HD12	1:D:1718:ALA:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:955:LYS:O	1:B:956:SER:OG	2.18	0.55
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: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:E:1729:GLU:O	1:E:1733:MET:HE3	2.06	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:1605:PHE:CE2	1:D:1664:MET:HE1	2.42	0.54
1:D:1994:GLU:N	1:D:1994:GLU:OE1	2.40	0.54
1:E:2057:TYR:OH	1:F:1877:ASN:O	2.20	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:C:1664:MET:HE2	1:C:1677:ILE:HD11	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1671:TYR:HH	1:F:1903:PRO:HA	1.73	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
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:D:1879:GLY:O	1:D:1964:MET:HE3	2.08	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:2098:SER:H	1:F:2107:MET:HE1	1.73	0.53
1:F:2319:ILE:HA	1:F:2322:MET:HB2	1.90	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:E:1882:HIS:HA	1:E:1964:MET:HE2	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:864:MET:HE1	1:B:1037:LYS:HA	1.90	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
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:F:1612:LEU:HD11	1:F:1616:MET:HE3	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:E:1605:PHE:CE2	1:E:1664:MET:HE1	2.44	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: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:1294:LYS:O	1:B:1295:THR:OG1	2.23	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:D:2286:SER:O	1:D:2286:SER:OG	2.18	0.52
1:E:863:VAL:HG21	1:E:881:TRP:HZ3	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:1870:GLY:HA2	1:E:1875:MET:HE2	1.91	0.52
1:D:1294:LYS:O	1:D:1295:THR:OG1	2.19	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:A:1288:ILE:C	1:A:1289:LEU:HD22	2.33	0.52
1:D:1235:GLY:O	1:D:1236:MET:HE3	2.09	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:A:884:ARG:O	1:A:888:THR:OG1	2.24	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: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:1755:PRO:HA	1:E:1758:TYR:CD1	2.46	0.50
1:E:2097:ASP:HA	1:E:2107:MET:HE1	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2232:ILE:O	1:C:2235:ALA:HB3	2.12	0.50
1:F:2022:SER:O	1:F:2026:THR:OG1	2.26	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:E:2264:TRP:O	1:E:2270:LEU:HD11	2.12	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
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: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:C:1483:MET:HE2	1:C:1487:LYS:HD2	1.93	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:D:1971:VAL:HG13	1:D:2025:LYS:HZ3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:2240:THR:HG1	1:D:2243:GLN:CD	2.13	0.49
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: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: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:1616:MET:CE	1:C:1897:HIS:HD1	2.26	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:C:1705:LEU:HD13	1:C:1705:LEU:C	2.39	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:980:ARG:HB3	1:D:983:MET:HE2	1.94	0.48
1:E:2093:TRP:CD1	1:F:1797:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1236:MET:HE3	1:E:1292:ALA:HB2	1.96	0.48
1:E:1923:ILE:HD13	1:E:1954:PHE:HA	1.94	0.48
1:C:1671:TYR:HH	1:C:1903:PRO:HA	1.79	0.48
1:C:1968:ALA:HB2	1:C:2021:ASP:HB2	1.94	0.48
1:B:1014:ARG:CZ	1:B:1021:MET:HE2	2.43	0.48
1:A:1301:ASP:OD1	1:A:1302:ASP:N	2.46	0.48
1:D:1937:MET:HE3	1:D:2043:PHE:HD2	1.77	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:1309:ARG:O	1:E:1312:THR:OG1	2.31	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:F:1386:MET:HE2	1:F:1424:ARG:HD2	1.95	0.48
1:E:991:LEU:HD12	1:E:992:ARG:HE	1.79	0.48
1:E:1632:LEU:HD12	1:E:1632:LEU:C	2.39	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:1471:ASN:HD22	1:E:1507:ARG:C	2.21	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: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:1791:GLY:C	1:F:1796:ASN:HD21	2.22	0.47
1:F:2110:ASP:O	1:F:2113:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1090:LEU:HD11	1:B:1096:ARG:NH1	2.29	0.47
1:A:682:VAL:C	1:A:683:LEU:HD12	2.39	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:B:682:VAL:C	1:B:683:LEU:HD12	2.39	0.47
1:A:705:ASP:N	1:A:705:ASP:OD1	2.46	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
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: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:1475:LEU:HD13	1:D:1475:LEU:C	2.39	0.47
1:D:2322:MET:SD	1:C:2308:VAL:HG11	2.54	0.47
1:E:913:ASN:OD1	1:E:913:ASN:N	2.47	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:C:2291:ASN:C	1:C:2295:ILE:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1699:PHE:O	1:C:1703:SER:OG	2.27	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
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:913:ASN:OD1	1:D:913:ASN:N	2.46	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:F:1705:LEU:C	1:F:1705:LEU:HD13	2.40	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:F:1616:MET:CE	1:F:1897:HIS:HD1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2150:ARG:O	1:C:2156:LEU:HD11	2.16	0.46
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:D:2315:ALA:HA	1:C:2322:MET:HE1	1.97	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:E:2116:SER:OG	1:E:2191:ASP:OD2	2.27	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:F:1616:MET:HE1	1:F:1897:HIS:HD1	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1664:MET:HE1	1:F:1679:VAL:HG12	1.97	0.46
1:B:980:ARG:O	1:B:984:LYS:NZ	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:983:MET:HE2	1:A:1051:ARG:CZ	2.46	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
1:A:964:ASN:O	1:A:968:ILE:HG22	2.16	0.46
1:A:1014:ARG:CZ	1:A:1021:MET:HE2	2.46	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:C:1995:LEU:C	1:C:1995:LEU:HD13	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1679:VAL:HG22	1:D:1714:ILE:CD1	2.38	0.45
1:E:2056:MET:HE1	1:E:2061:LEU:HD21	1.97	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:F:1995:LEU:HD13	1:F:1995:LEU:C	2.42	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:705:ASP:OD1	1:B:705:ASP:N	2.49	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:705:ASP:OD1	1:A:717:SER:OG	2.17	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
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:1154:VAL:HG13	1:A:1180:PHE:CE1	2.52	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:C:1847:ILE:C	1:C:1848:LEU:HD22	2.42	0.45
1:F:1671:TYR:OH	1:F:1903:PRO:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1860:ARG:HH21	1:F:2004:LEU:HD21	1.81	0.45
1:F:1901:TYR:C	1:F:1902:MET:HE2	2.42	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: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:1249:PHE:CE2	1:E:1253:MET:HE3	2.52	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
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:1901:TYR:HB2	1:C:1902:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:903:MET:HE1	1:E:910:ILE:HD13	1.98	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:E:2223:LEU:C	1:E:2223:LEU:HD13	2.43	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:D:2223:LEU:HD13	1:D:2223:LEU:C	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2278:LEU:C	1:D:2278:LEU:HD13	2.43	0.44
1:E:625:ARG:HB3	1:E:626:PRO:CD	2.48	0.44
1:E:1937:MET:HE3	1:E:2043:PHE:HD2	1.83	0.44
1:E:2068:VAL:HG21	1:E:2095:VAL:HG12	2.00	0.44
1:F:1539:TYR:HH	1:F:1606:ARG:NH1	2.15	0.44
1:F:1999:ALA:HB2	1:F:2007:GLU:C	2.43	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:D:1932:TYR:H	1:D:1990:THR:HG1	1.64	0.43
1:D:2097:ASP:HA	1:D:2107:MET:HE1	2.00	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:F:1480:THR:OG1	1:F:1480:THR:O	2.35	0.43
1:A:1492:VAL:O	1:A:1496:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:886:MET:HE1	1:B:1047:GLN:HB2	1.99	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1809:LEU:HD23	1:E:1809:LEU:C	2.43	0.43
1:C:1999:ALA:HB2	1:C:2007:GLU:C	2.43	0.43
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:E:2219:LEU:C	1:E:2219:LEU:HD13	2.44	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: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: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:F:1677:ILE:HD12	1:F:1677:ILE:C	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2053:MET:HB2	1:F:1863:TYR:CE1	2.54	0.43
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:D:918:ILE:HD12	1:D:922:MET:HE3	2.01	0.42
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: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:1639:LEU:HD21	1:D:1643:GLY:C	2.45	0.42
1:E:918:ILE:HD12	1:E:922:MET:HE3	2.00	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:F:2087:GLU:C	1:F:2088:LEU:HD22	2.44	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:2098:SER:HA	1:D:2105:MET:HE2	2.01	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:E:2039:PRO:C	1:E:2040:LEU:HD22	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1126:SER:OG	1:B:1128:THR:O	2.30	0.42
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:C:2041:MET:HE3	1:C:2079:LEU:HD12	2.01	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:F:1664:MET:HE1	1:F:1679:VAL:CG1	2.49	0.42
1:F:2325:HIS:C	1:F:2327:SER:H	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:1750:TYR:OH	1:D:1774:ASP:OD2	2.27	0.41
1:E:1048:LEU:C	1:E:1048:LEU:HD23	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1483:MET:H	1:D:1517:ILE:HD11	1.84	0.41
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:E:1815:ILE:HD11	1:E:2036:GLU:CD	2.45	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:1180:PHE:CZ	1:D:1236:MET:HE1	2.55	0.41
1:D:1405:LEU:C	1:D:1405:LEU:HD23	2.45	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:D:1243:GLU:C	1:D:1247:ARG:HE	2.28	0.41
1:D:1540:LEU:HD12	1:D:1540:LEU:C	2.46	0.41
1:D:2219:LEU:HD13	1:D:2219:LEU:C	2.45	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:1528:ILE:O	1:D:1528:ILE:HG22	2.19	0.41
1:D:1534:ASN:HD22	1:D:1535:GLU:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2227:LEU:HD13	1:D:2227:LEU:C	2.46	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:F:2119:GLU:CD	1:F:2121:GLU:HG2	2.45	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:1596:THR:OG1	1:D:1888:ASP:OD2	2.21	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
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: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:1330:LEU:C	1:D:1330:LEU:HD23	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1483:MET:HE2	1:A:1488:ILE:CG1	2.51	0.41
1:D:2053:MET:HB2	1:C:1863:TYR:CE1	2.55	0.41
1:D:2057:TYR:C	1:C:1878:ASN:HD22	2.26	0.41
1:E:2108:TYR:OH	1:E:2218:ARG:NH2	2.49	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: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:F:2231:LYS:HZ2	1:F:2292:ILE:HD13	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1025:LEU:C	1:D:1025:LEU:HD23	2.47	0.40
1:D:1249:PHE:CE2	1:D:1253:MET:HE3	2.57	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
1:D:848:LYS:O	1:D:852:VAL:HG23	2.21	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:1659:MET:HE2	1:F:1695:GLU:HB3	2.03	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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/2407 (31%)	640 (86%)	93 (13%)	8 (1%)	11	45
1	B	741/2407 (31%)	641 (86%)	93 (13%)	7 (1%)	14	49
1	C	940/2407 (39%)	882 (94%)	51 (5%)	7 (1%)	18	55
1	D	1498/2407 (62%)	1367 (91%)	123 (8%)	8 (0%)	24	63
1	E	1498/2407 (62%)	1371 (92%)	117 (8%)	10 (1%)	18	55
1	F	940/2407 (39%)	883 (94%)	51 (5%)	6 (1%)	21	58
All	All	6358/14442 (44%)	5784 (91%)	528 (8%)	46 (1%)	20	55

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	673 (97%)	21 (3%)	36	57
1	B	694/2108 (33%)	676 (97%)	18 (3%)	40	60
1	C	830/2108 (39%)	813 (98%)	17 (2%)	48	65
1	D	1354/2108 (64%)	1323 (98%)	31 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1354/2108 (64%)	1322 (98%)	32 (2%)	43	63
1	F	830/2108 (39%)	817 (98%)	13 (2%)	55	69
All	All	5756/12648 (46%)	5624 (98%)	132 (2%)	44	63

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	863	VAL
1	D	889	LEU
1	D	944	ILE
1	D	947	SER
1	D	951	THR
1	D	986	VAL
1	D	995	LEU
1	D	1055	LEU
1	D	1079	LEU
1	D	1095	LEU
1	D	1105	LEU
1	D	1175	THR
1	D	1236	MET
1	D	1373	LEU
1	D	1381	LEU
1	D	1403	LEU
1	D	1438	SER
1	D	1449	LEU
1	D	1450	LEU
1	D	1470	CYS
1	D	1480	THR
1	D	1508	VAL
1	D	1540	LEU
1	D	1649	ASN
1	D	1797	LEU
1	D	1915	SER
1	D	1919	ILE
1	D	2116	SER
1	D	2124	VAL
1	D	2176	ILE
1	D	2327	SER
1	E	644	LEU
1	E	674	LEU
1	E	734	TYR

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Mol	Chain	Res	Type
1	E	860	LEU
1	E	863	VAL
1	E	875	SER
1	E	889	LEU
1	E	947	SER
1	E	951	THR
1	E	990	LEU
1	E	1060	LEU
1	E	1085	LEU
1	E	1095	LEU
1	E	1105	LEU
1	E	1125	LEU
1	E	1175	THR
1	E	1381	LEU
1	E	1391	LEU
1	E	1438	SER
1	E	1449	LEU
1	E	1451	LEU
1	E	1480	THR
1	E	1508	VAL
1	E	1528	ILE
1	E	1571	MET
1	E	1649	ASN
1	E	1919	ILE
1	E	2067	ILE
1	E	2116	SER
1	E	2124	VAL
1	E	2176	ILE
1	E	2327	SER
1	C	1381	LEU
1	C	1384	ASN
1	C	1438	SER
1	C	1478	VAL
1	C	1480	THR
1	C	1526	ILE
1	C	1541	ASP
1	C	1601	ILE
1	C	1622	LEU
1	C	1649	ASN
1	C	1705	LEU
1	C	1848	LEU
1	C	1902	MET

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Mol	Chain	Res	Type
1	C	2116	SER
1	C	2168	LEU
1	C	2240	THR
1	C	2327	SER
1	F	1381	LEU
1	F	1438	SER
1	F	1478	VAL
1	F	1480	THR
1	F	1508	VAL
1	F	1526	ILE
1	F	1601	ILE
1	F	1649	ASN
1	F	1705	LEU
1	F	2116	SER
1	F	2206	LEU
1	F	2240	THR
1	F	2327	SER
1	B	637	LEU
1	B	863	VAL
1	B	897	LEU
1	B	951	THR
1	B	986	VAL
1	B	995	LEU
1	B	1105	LEU
1	B	1164	ASN
1	B	1175	THR
1	B	1233	MET
1	B	1250	ASP
1	B	1377	LEU
1	B	1381	LEU
1	B	1414	THR
1	B	1438	SER
1	B	1457	LEU
1	B	1514	LYS
1	B	1528	ILE
1	A	637	LEU
1	A	655	LEU
1	A	734	TYR
1	A	862	ASN
1	A	863	VAL
1	A	897	LEU
1	A	947	SER

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Mol	Chain	Res	Type
1	A	951	THR
1	A	986	VAL
1	A	995	LEU
1	A	1034	VAL
1	A	1105	LEU
1	A	1164	ASN
1	A	1175	THR
1	A	1377	LEU
1	A	1381	LEU
1	A	1438	SER
1	A	1457	LEU
1	A	1480	THR
1	A	1514	LYS
1	A	1528	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	638	HIS
1	D	653	HIS
1	D	668	ASN
1	D	939	GLN
1	D	1000	GLN
1	D	1022	ASN
1	D	1114	GLN
1	D	1119	ASN
1	D	1315	ASN
1	D	1402	HIS
1	D	1443	GLN
1	D	1444	ASN
1	D	1471	ASN
1	D	1574	ASN
1	D	1589	GLN
1	D	1647	HIS
1	D	1649	ASN
1	D	1655	ASN
1	D	1771	HIS
1	D	1840	GLN
1	D	2003	ASN
1	D	2045	ASN
1	D	2059	GLN
1	D	2085	GLN

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Mol	Chain	Res	Type
1	D	2146	HIS
1	D	2267	ASN
1	D	2291	ASN
1	E	638	HIS
1	E	653	HIS
1	E	850	HIS
1	E	862	ASN
1	E	940	GLN
1	E	964	ASN
1	E	1005	HIS
1	E	1022	ASN
1	E	1061	ASN
1	E	1083	GLN
1	E	1099	GLN
1	E	1181	GLN
1	E	1399	HIS
1	E	1402	HIS
1	E	1443	GLN
1	E	1444	ASN
1	E	1510	GLN
1	E	1589	GLN
1	E	1649	ASN
1	E	1682	ASN
1	E	1771	HIS
1	E	1969	GLN
1	E	2003	ASN
1	E	2013	GLN
1	E	2034	ASN
1	E	2059	GLN
1	E	2085	GLN
1	E	2146	HIS
1	E	2243	GLN
1	E	2245	GLN
1	E	2291	ASN
1	E	2321	HIS
1	C	1398	ASN
1	C	1402	HIS
1	C	1534	ASN
1	C	1569	HIS
1	C	1965	GLN
1	C	2003	ASN
1	C	2016	GLN

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Mol	Chain	Res	Type
1	C	2076	GLN
1	C	2180	HIS
1	C	2181	GLN
1	C	2325	HIS
1	F	1402	HIS
1	F	1534	ASN
1	F	1565	GLN
1	F	1569	HIS
1	F	1649	ASN
1	F	1796	ASN
1	F	1812	ASN
1	F	1965	GLN
1	F	2003	ASN
1	F	2076	GLN
1	F	2181	GLN
1	F	2243	GLN
1	F	2277	GLN
1	F	2303	GLN
1	F	2325	HIS
1	B	650	ASN
1	B	653	HIS
1	B	668	ASN
1	B	928	ASN
1	B	966	GLN
1	B	973	GLN
1	B	1026	ASN
1	B	1068	GLN
1	B	1083	GLN
1	B	1113	HIS
1	B	1136	ASN
1	B	1181	GLN
1	B	1314	GLN
1	B	1534	ASN
1	A	650	ASN
1	A	668	ASN
1	A	939	GLN
1	A	966	GLN
1	A	973	GLN
1	A	982	HIS
1	A	1005	HIS
1	A	1026	ASN
1	A	1113	HIS

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Mol	Chain	Res	Type
1	A	1290	ASN
1	A	1315	ASN
1	A	1388	ASN
1	A	1534	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

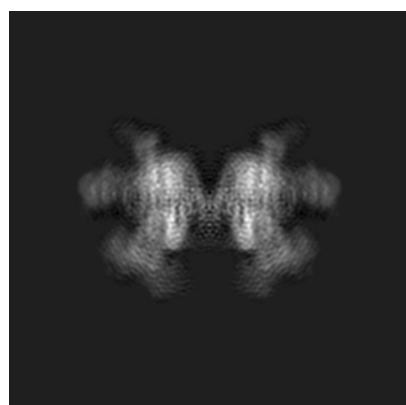
6 Map visualisation [i](#)

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

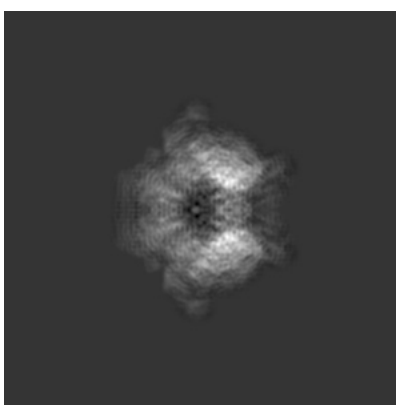
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

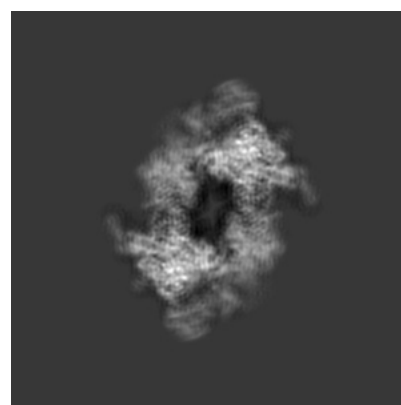
6.1.1 Primary map



X



Y

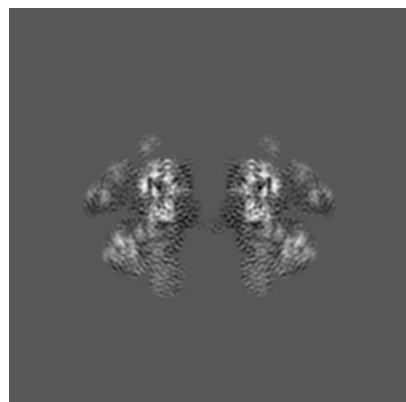


Z

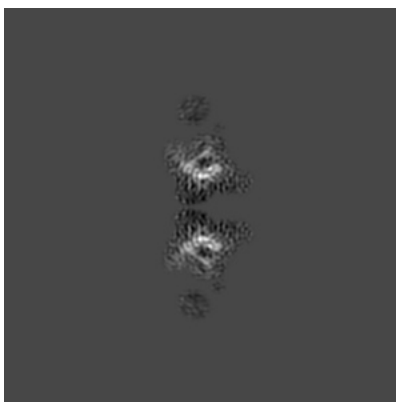
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

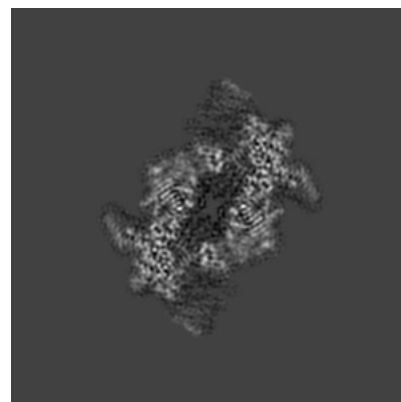
6.2.1 Primary map



X Index: 188



Y Index: 188

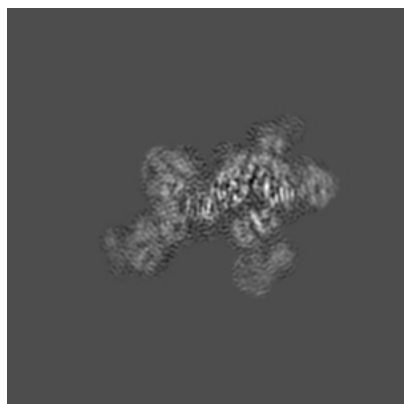


Z Index: 188

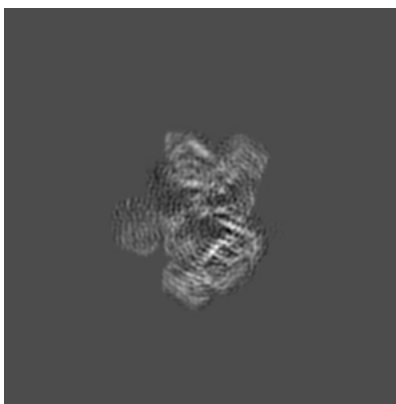
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

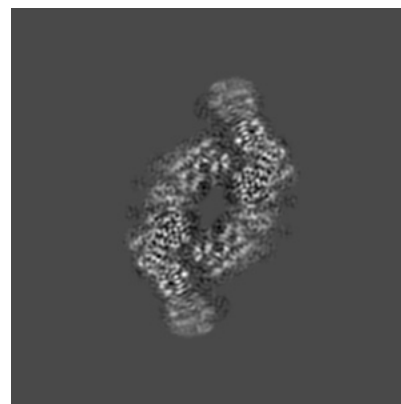
6.3.1 Primary map



X Index: 219



Y Index: 153

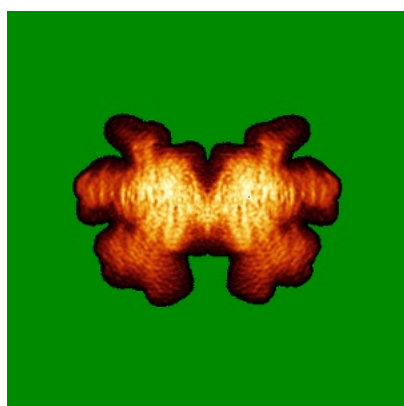


Z Index: 201

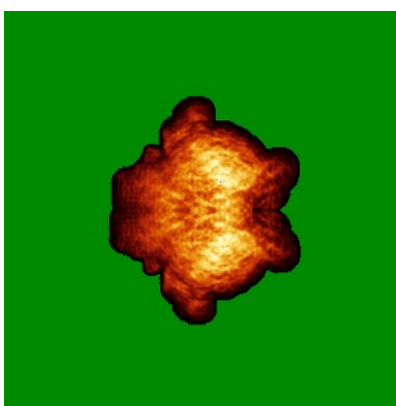
The images above show the largest variance slices of the map in three orthogonal directions.

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

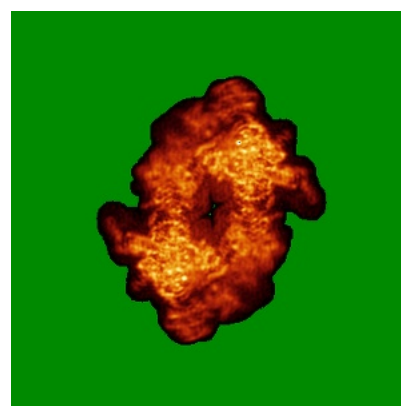
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

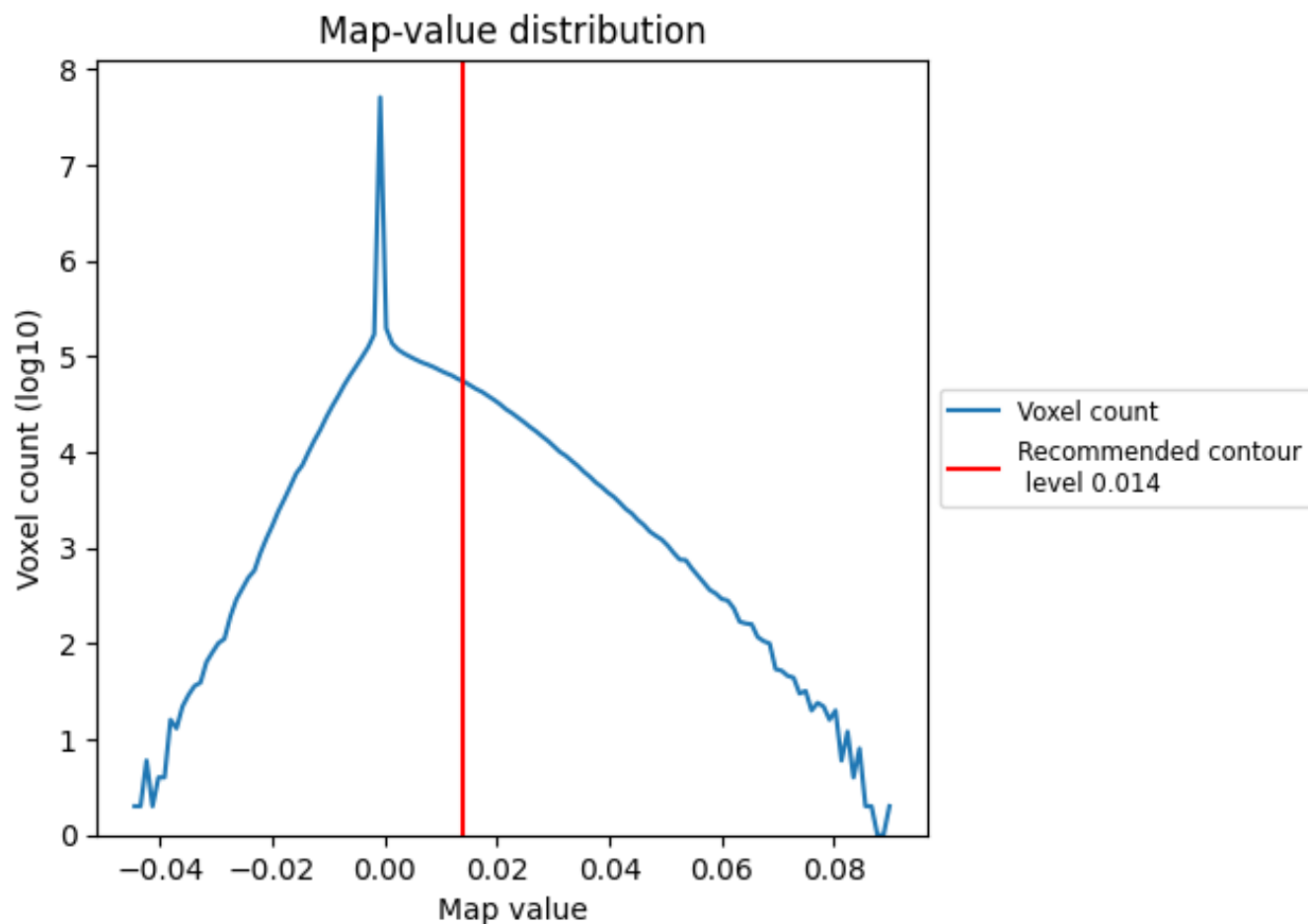
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

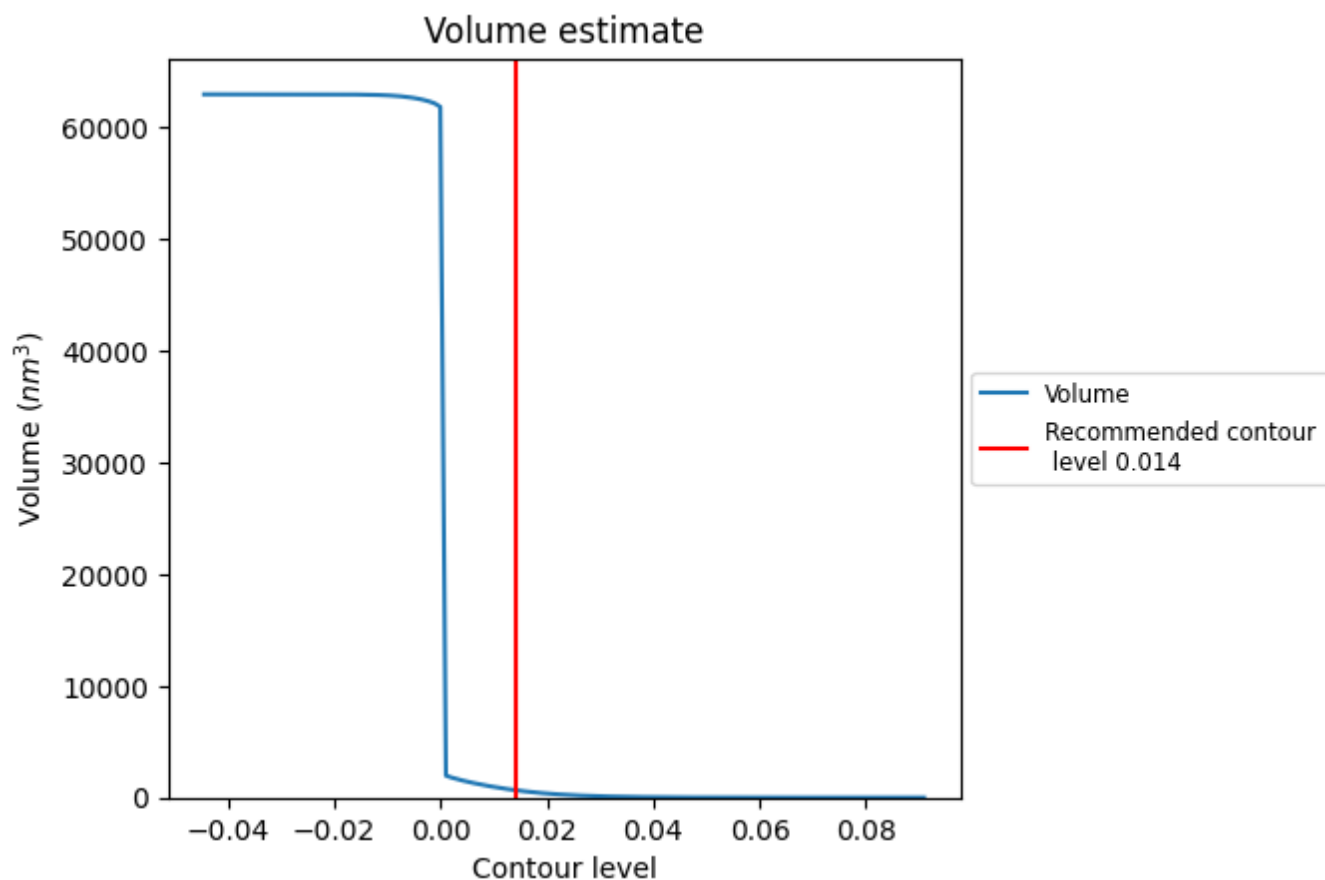
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

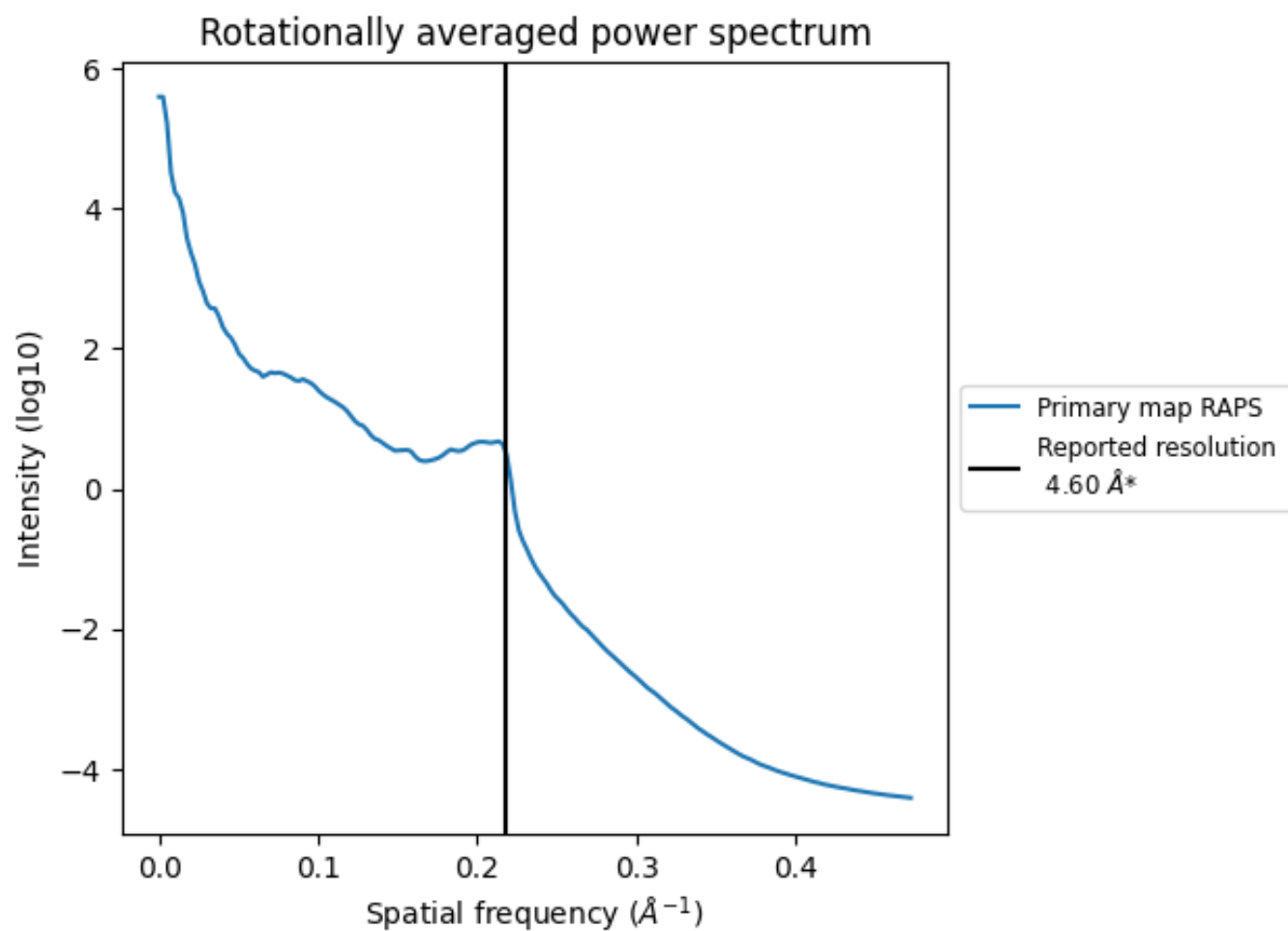
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 664 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

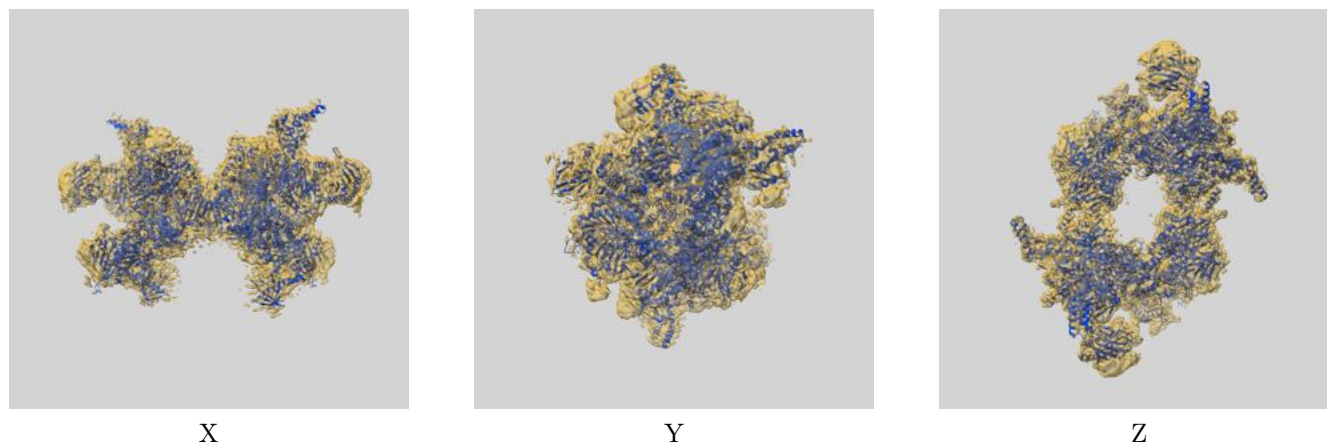
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

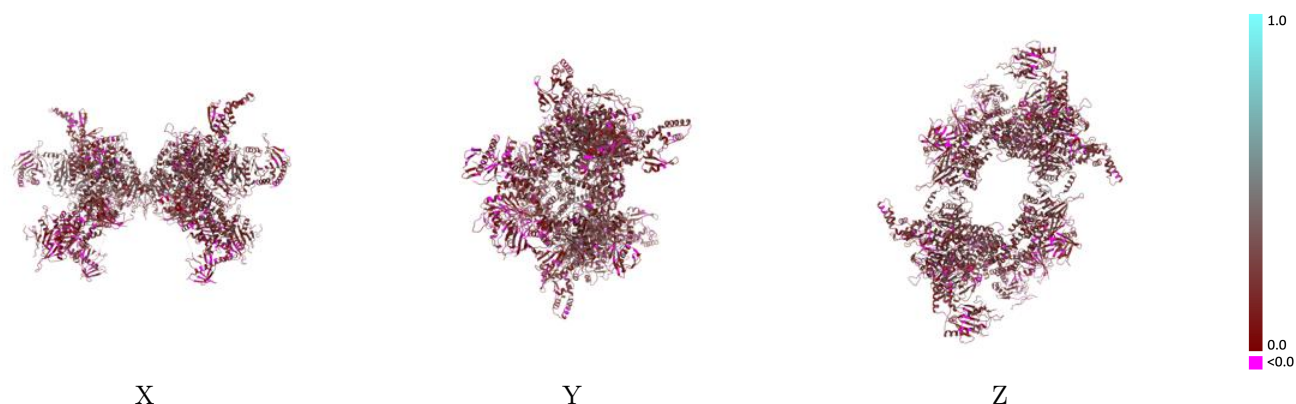
This section contains information regarding the fit between EMDB map EMD-4343 and PDB model 6G2H. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



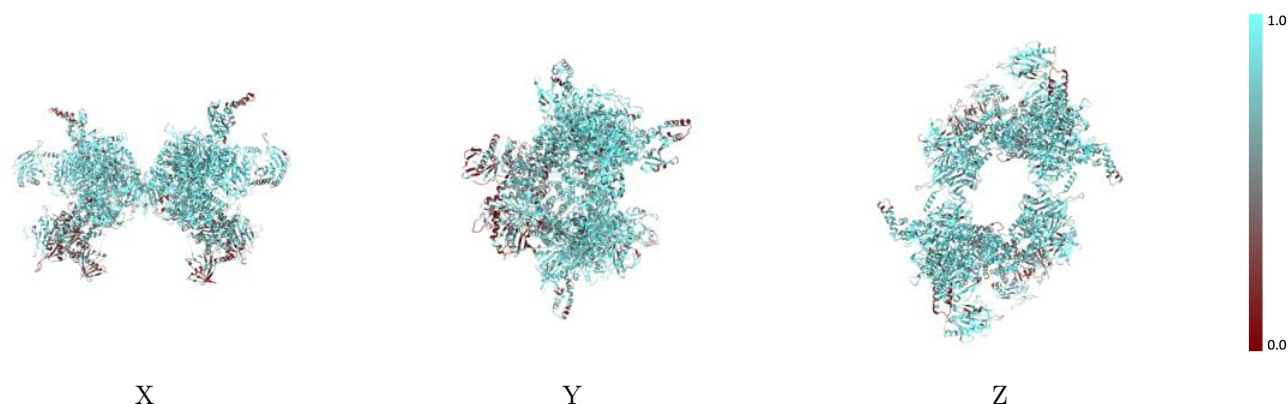
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



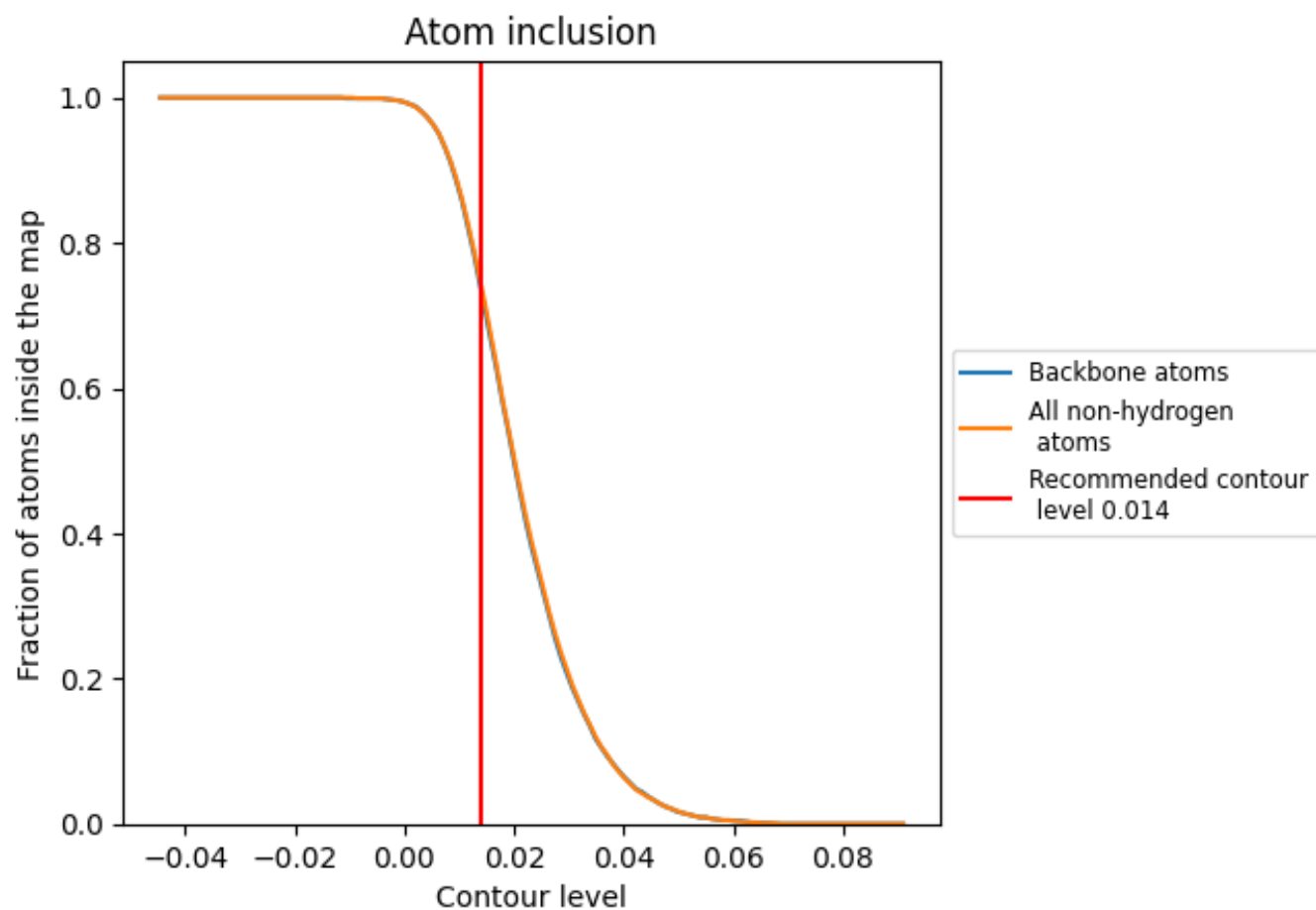
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

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	0.7410	0.2070
A	0.5560	0.1510
B	0.5520	0.1490
C	0.8000	0.2210
D	0.8040	0.2250
E	0.8040	0.2280
F	0.7990	0.2210

1.0

0.0

<0.0