



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:07 AM UTC

PDB ID : 9IY6 / pdb\_00009iy6  
EMDB ID : EMD-60986  
Title : BTN2A1-BTN3A1-BTN3A2 oligomer complex  
Authors : Xin, W.; Huang, B.; Su, Q.; Zhou, Q.  
Deposited on : 2024-07-30  
Resolution : 10.00 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](mailto: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>.

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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

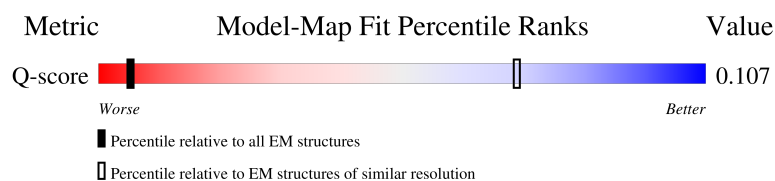
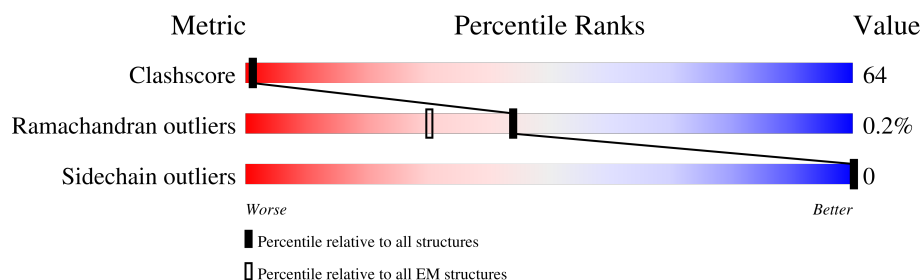
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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	147 ( 9.50 - 10.50 )

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  $\geq 3$ , 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	E	534	
1	F	534	
1	I	534	
1	J	534	

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Mol	Chain	Length	Quality of chain
2	G	340	<div><div><div></div><div></div><div></div></div><div>25%38%36%</div></div>
2	K	340	<div><div><div></div><div></div><div></div></div><div>22%41%36%</div></div>
3	H	539	<div><div><div></div><div></div><div></div></div><div>14%23%17%60%</div></div>
3	L	539	<div><div><div></div><div></div><div></div></div><div>12%28%60%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13310 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	F	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	I	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	J	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	7	MET	-	initiating methionine	UNP Q7KYR7
E	8	ASP	-	expression tag	UNP Q7KYR7
E	9	MET	-	expression tag	UNP Q7KYR7
E	10	ARG	-	expression tag	UNP Q7KYR7
E	11	VAL	-	expression tag	UNP Q7KYR7
E	12	PRO	-	expression tag	UNP Q7KYR7
E	13	ALA	-	expression tag	UNP Q7KYR7
E	14	GLN	-	expression tag	UNP Q7KYR7
E	15	LEU	-	expression tag	UNP Q7KYR7
E	16	LEU	-	expression tag	UNP Q7KYR7
E	17	GLY	-	expression tag	UNP Q7KYR7
E	18	LEU	-	expression tag	UNP Q7KYR7
E	19	LEU	-	expression tag	UNP Q7KYR7
E	20	LEU	-	expression tag	UNP Q7KYR7
E	21	LEU	-	expression tag	UNP Q7KYR7
E	22	TRP	-	expression tag	UNP Q7KYR7
E	23	LEU	-	expression tag	UNP Q7KYR7
E	24	SER	-	expression tag	UNP Q7KYR7
E	25	GLY	-	expression tag	UNP Q7KYR7
E	26	ALA	-	expression tag	UNP Q7KYR7
E	27	ARG	-	expression tag	UNP Q7KYR7
E	28	CYS	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	528	GLY	-	expression tag	UNP Q7KYR7
E	529	SER	-	expression tag	UNP Q7KYR7
E	530	SER	-	expression tag	UNP Q7KYR7
E	531	GLY	-	expression tag	UNP Q7KYR7
E	532	MET	-	expression tag	UNP Q7KYR7
E	533	ASP	-	expression tag	UNP Q7KYR7
E	534	TYR	-	expression tag	UNP Q7KYR7
E	535	LYS	-	expression tag	UNP Q7KYR7
E	536	ASP	-	expression tag	UNP Q7KYR7
E	537	ASP	-	expression tag	UNP Q7KYR7
E	538	ASP	-	expression tag	UNP Q7KYR7
E	539	ASP	-	expression tag	UNP Q7KYR7
E	540	LYS	-	expression tag	UNP Q7KYR7
F	7	MET	-	initiating methionine	UNP Q7KYR7
F	8	ASP	-	expression tag	UNP Q7KYR7
F	9	MET	-	expression tag	UNP Q7KYR7
F	10	ARG	-	expression tag	UNP Q7KYR7
F	11	VAL	-	expression tag	UNP Q7KYR7
F	12	PRO	-	expression tag	UNP Q7KYR7
F	13	ALA	-	expression tag	UNP Q7KYR7
F	14	GLN	-	expression tag	UNP Q7KYR7
F	15	LEU	-	expression tag	UNP Q7KYR7
F	16	LEU	-	expression tag	UNP Q7KYR7
F	17	GLY	-	expression tag	UNP Q7KYR7
F	18	LEU	-	expression tag	UNP Q7KYR7
F	19	LEU	-	expression tag	UNP Q7KYR7
F	20	LEU	-	expression tag	UNP Q7KYR7
F	21	LEU	-	expression tag	UNP Q7KYR7
F	22	TRP	-	expression tag	UNP Q7KYR7
F	23	LEU	-	expression tag	UNP Q7KYR7
F	24	SER	-	expression tag	UNP Q7KYR7
F	25	GLY	-	expression tag	UNP Q7KYR7
F	26	ALA	-	expression tag	UNP Q7KYR7
F	27	ARG	-	expression tag	UNP Q7KYR7
F	28	CYS	-	expression tag	UNP Q7KYR7
F	528	GLY	-	expression tag	UNP Q7KYR7
F	529	SER	-	expression tag	UNP Q7KYR7
F	530	SER	-	expression tag	UNP Q7KYR7
F	531	GLY	-	expression tag	UNP Q7KYR7
F	532	MET	-	expression tag	UNP Q7KYR7
F	533	ASP	-	expression tag	UNP Q7KYR7
F	534	TYR	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	535	LYS	-	expression tag	UNP Q7KYR7
F	536	ASP	-	expression tag	UNP Q7KYR7
F	537	ASP	-	expression tag	UNP Q7KYR7
F	538	ASP	-	expression tag	UNP Q7KYR7
F	539	ASP	-	expression tag	UNP Q7KYR7
F	540	LYS	-	expression tag	UNP Q7KYR7
I	7	MET	-	initiating methionine	UNP Q7KYR7
I	8	ASP	-	expression tag	UNP Q7KYR7
I	9	MET	-	expression tag	UNP Q7KYR7
I	10	ARG	-	expression tag	UNP Q7KYR7
I	11	VAL	-	expression tag	UNP Q7KYR7
I	12	PRO	-	expression tag	UNP Q7KYR7
I	13	ALA	-	expression tag	UNP Q7KYR7
I	14	GLN	-	expression tag	UNP Q7KYR7
I	15	LEU	-	expression tag	UNP Q7KYR7
I	16	LEU	-	expression tag	UNP Q7KYR7
I	17	GLY	-	expression tag	UNP Q7KYR7
I	18	LEU	-	expression tag	UNP Q7KYR7
I	19	LEU	-	expression tag	UNP Q7KYR7
I	20	LEU	-	expression tag	UNP Q7KYR7
I	21	LEU	-	expression tag	UNP Q7KYR7
I	22	TRP	-	expression tag	UNP Q7KYR7
I	23	LEU	-	expression tag	UNP Q7KYR7
I	24	SER	-	expression tag	UNP Q7KYR7
I	25	GLY	-	expression tag	UNP Q7KYR7
I	26	ALA	-	expression tag	UNP Q7KYR7
I	27	ARG	-	expression tag	UNP Q7KYR7
I	28	CYS	-	expression tag	UNP Q7KYR7
I	528	GLY	-	expression tag	UNP Q7KYR7
I	529	SER	-	expression tag	UNP Q7KYR7
I	530	SER	-	expression tag	UNP Q7KYR7
I	531	GLY	-	expression tag	UNP Q7KYR7
I	532	MET	-	expression tag	UNP Q7KYR7
I	533	ASP	-	expression tag	UNP Q7KYR7
I	534	TYR	-	expression tag	UNP Q7KYR7
I	535	LYS	-	expression tag	UNP Q7KYR7
I	536	ASP	-	expression tag	UNP Q7KYR7
I	537	ASP	-	expression tag	UNP Q7KYR7
I	538	ASP	-	expression tag	UNP Q7KYR7
I	539	ASP	-	expression tag	UNP Q7KYR7
I	540	LYS	-	expression tag	UNP Q7KYR7
J	7	MET	-	initiating methionine	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	8	ASP	-	expression tag	UNP Q7KYR7
J	9	MET	-	expression tag	UNP Q7KYR7
J	10	ARG	-	expression tag	UNP Q7KYR7
J	11	VAL	-	expression tag	UNP Q7KYR7
J	12	PRO	-	expression tag	UNP Q7KYR7
J	13	ALA	-	expression tag	UNP Q7KYR7
J	14	GLN	-	expression tag	UNP Q7KYR7
J	15	LEU	-	expression tag	UNP Q7KYR7
J	16	LEU	-	expression tag	UNP Q7KYR7
J	17	GLY	-	expression tag	UNP Q7KYR7
J	18	LEU	-	expression tag	UNP Q7KYR7
J	19	LEU	-	expression tag	UNP Q7KYR7
J	20	LEU	-	expression tag	UNP Q7KYR7
J	21	LEU	-	expression tag	UNP Q7KYR7
J	22	TRP	-	expression tag	UNP Q7KYR7
J	23	LEU	-	expression tag	UNP Q7KYR7
J	24	SER	-	expression tag	UNP Q7KYR7
J	25	GLY	-	expression tag	UNP Q7KYR7
J	26	ALA	-	expression tag	UNP Q7KYR7
J	27	ARG	-	expression tag	UNP Q7KYR7
J	28	CYS	-	expression tag	UNP Q7KYR7
J	528	GLY	-	expression tag	UNP Q7KYR7
J	529	SER	-	expression tag	UNP Q7KYR7
J	530	SER	-	expression tag	UNP Q7KYR7
J	531	GLY	-	expression tag	UNP Q7KYR7
J	532	MET	-	expression tag	UNP Q7KYR7
J	533	ASP	-	expression tag	UNP Q7KYR7
J	534	TYR	-	expression tag	UNP Q7KYR7
J	535	LYS	-	expression tag	UNP Q7KYR7
J	536	ASP	-	expression tag	UNP Q7KYR7
J	537	ASP	-	expression tag	UNP Q7KYR7
J	538	ASP	-	expression tag	UNP Q7KYR7
J	539	ASP	-	expression tag	UNP Q7KYR7
J	540	LYS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	216	Total	C	N	O	S	0	0
			1630	1027	279	316	8		
2	K	216	Total	C	N	O	S	0	0
			1630	1027	279	316	8		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	MET	-	initiating methionine	UNP P78410
G	9	ASP	-	expression tag	UNP P78410
G	10	MET	-	expression tag	UNP P78410
G	11	ARG	-	expression tag	UNP P78410
G	12	VAL	-	expression tag	UNP P78410
G	13	PRO	-	expression tag	UNP P78410
G	14	ALA	-	expression tag	UNP P78410
G	15	GLN	-	expression tag	UNP P78410
G	16	LEU	-	expression tag	UNP P78410
G	17	LEU	-	expression tag	UNP P78410
G	18	GLY	-	expression tag	UNP P78410
G	19	LEU	-	expression tag	UNP P78410
G	20	LEU	-	expression tag	UNP P78410
G	21	LEU	-	expression tag	UNP P78410
G	22	LEU	-	expression tag	UNP P78410
G	23	TRP	-	expression tag	UNP P78410
G	24	LEU	-	expression tag	UNP P78410
G	25	SER	-	expression tag	UNP P78410
G	26	GLY	-	expression tag	UNP P78410
G	27	ALA	-	expression tag	UNP P78410
G	28	ARG	-	expression tag	UNP P78410
G	29	CYS	-	expression tag	UNP P78410
G	335	GLY	-	expression tag	UNP P78410
G	336	SER	-	expression tag	UNP P78410
G	337	SER	-	expression tag	UNP P78410
G	338	GLY	-	expression tag	UNP P78410
G	339	MET	-	expression tag	UNP P78410
G	340	ASP	-	expression tag	UNP P78410
G	341	TYR	-	expression tag	UNP P78410
G	342	LYS	-	expression tag	UNP P78410
G	343	ASP	-	expression tag	UNP P78410
G	344	ASP	-	expression tag	UNP P78410
G	345	ASP	-	expression tag	UNP P78410
G	346	ASP	-	expression tag	UNP P78410
G	347	LYS	-	expression tag	UNP P78410
K	8	MET	-	initiating methionine	UNP P78410
K	9	ASP	-	expression tag	UNP P78410
K	10	MET	-	expression tag	UNP P78410
K	11	ARG	-	expression tag	UNP P78410
K	12	VAL	-	expression tag	UNP P78410
K	13	PRO	-	expression tag	UNP P78410
K	14	ALA	-	expression tag	UNP P78410

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Chain	Residue	Modelled	Actual	Comment	Reference
K	15	GLN	-	expression tag	UNP P78410
K	16	LEU	-	expression tag	UNP P78410
K	17	LEU	-	expression tag	UNP P78410
K	18	GLY	-	expression tag	UNP P78410
K	19	LEU	-	expression tag	UNP P78410
K	20	LEU	-	expression tag	UNP P78410
K	21	LEU	-	expression tag	UNP P78410
K	22	LEU	-	expression tag	UNP P78410
K	23	TRP	-	expression tag	UNP P78410
K	24	LEU	-	expression tag	UNP P78410
K	25	SER	-	expression tag	UNP P78410
K	26	GLY	-	expression tag	UNP P78410
K	27	ALA	-	expression tag	UNP P78410
K	28	ARG	-	expression tag	UNP P78410
K	29	CYS	-	expression tag	UNP P78410
K	335	GLY	-	expression tag	UNP P78410
K	336	SER	-	expression tag	UNP P78410
K	337	SER	-	expression tag	UNP P78410
K	338	GLY	-	expression tag	UNP P78410
K	339	MET	-	expression tag	UNP P78410
K	340	ASP	-	expression tag	UNP P78410
K	341	TYR	-	expression tag	UNP P78410
K	342	LYS	-	expression tag	UNP P78410
K	343	ASP	-	expression tag	UNP P78410
K	344	ASP	-	expression tag	UNP P78410
K	345	ASP	-	expression tag	UNP P78410
K	346	ASP	-	expression tag	UNP P78410
K	347	LYS	-	expression tag	UNP P78410

- Molecule 3 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	216	Total	C	N	O	S	0	0
			1629	1025	279	317	8		
3	L	216	Total	C	N	O	S	0	0
			1629	1025	279	317	8		

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	MET	-	initiating methionine	UNP O00481
H	9	ASP	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
H	10	MET	-	expression tag	UNP O00481
H	11	ARG	-	expression tag	UNP O00481
H	12	VAL	-	expression tag	UNP O00481
H	13	PRO	-	expression tag	UNP O00481
H	14	ALA	-	expression tag	UNP O00481
H	15	GLN	-	expression tag	UNP O00481
H	16	LEU	-	expression tag	UNP O00481
H	17	LEU	-	expression tag	UNP O00481
H	18	GLY	-	expression tag	UNP O00481
H	19	LEU	-	expression tag	UNP O00481
H	20	LEU	-	expression tag	UNP O00481
H	21	LEU	-	expression tag	UNP O00481
H	22	LEU	-	expression tag	UNP O00481
H	23	TRP	-	expression tag	UNP O00481
H	24	LEU	-	expression tag	UNP O00481
H	25	SER	-	expression tag	UNP O00481
H	26	GLY	-	expression tag	UNP O00481
H	27	ALA	-	expression tag	UNP O00481
H	28	ARG	-	expression tag	UNP O00481
H	29	CYS	-	expression tag	UNP O00481
H	514	GLY	-	expression tag	UNP O00481
H	515	SER	-	expression tag	UNP O00481
H	516	SER	-	expression tag	UNP O00481
H	517	GLY	-	expression tag	UNP O00481
H	518	ALA	-	expression tag	UNP O00481
H	519	TRP	-	expression tag	UNP O00481
H	520	SER	-	expression tag	UNP O00481
H	521	HIS	-	expression tag	UNP O00481
H	522	PRO	-	expression tag	UNP O00481
H	523	GLN	-	expression tag	UNP O00481
H	524	PHE	-	expression tag	UNP O00481
H	525	GLU	-	expression tag	UNP O00481
H	526	LYS	-	expression tag	UNP O00481
H	527	GLY	-	expression tag	UNP O00481
H	528	GLY	-	expression tag	UNP O00481
H	529	GLY	-	expression tag	UNP O00481
H	530	SER	-	expression tag	UNP O00481
H	531	GLY	-	expression tag	UNP O00481
H	532	GLY	-	expression tag	UNP O00481
H	533	GLY	-	expression tag	UNP O00481
H	534	SER	-	expression tag	UNP O00481
H	535	GLY	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
H	536	GLY	-	expression tag	UNP O00481
H	537	SER	-	expression tag	UNP O00481
H	538	ALA	-	expression tag	UNP O00481
H	539	TRP	-	expression tag	UNP O00481
H	540	SER	-	expression tag	UNP O00481
H	541	HIS	-	expression tag	UNP O00481
H	542	PRO	-	expression tag	UNP O00481
H	543	GLN	-	expression tag	UNP O00481
H	544	PHE	-	expression tag	UNP O00481
H	545	GLU	-	expression tag	UNP O00481
H	546	LYS	-	expression tag	UNP O00481
L	8	MET	-	initiating methionine	UNP O00481
L	9	ASP	-	expression tag	UNP O00481
L	10	MET	-	expression tag	UNP O00481
L	11	ARG	-	expression tag	UNP O00481
L	12	VAL	-	expression tag	UNP O00481
L	13	PRO	-	expression tag	UNP O00481
L	14	ALA	-	expression tag	UNP O00481
L	15	GLN	-	expression tag	UNP O00481
L	16	LEU	-	expression tag	UNP O00481
L	17	LEU	-	expression tag	UNP O00481
L	18	GLY	-	expression tag	UNP O00481
L	19	LEU	-	expression tag	UNP O00481
L	20	LEU	-	expression tag	UNP O00481
L	21	LEU	-	expression tag	UNP O00481
L	22	LEU	-	expression tag	UNP O00481
L	23	TRP	-	expression tag	UNP O00481
L	24	LEU	-	expression tag	UNP O00481
L	25	SER	-	expression tag	UNP O00481
L	26	GLY	-	expression tag	UNP O00481
L	27	ALA	-	expression tag	UNP O00481
L	28	ARG	-	expression tag	UNP O00481
L	29	CYS	-	expression tag	UNP O00481
L	514	GLY	-	expression tag	UNP O00481
L	515	SER	-	expression tag	UNP O00481
L	516	SER	-	expression tag	UNP O00481
L	517	GLY	-	expression tag	UNP O00481
L	518	ALA	-	expression tag	UNP O00481
L	519	TRP	-	expression tag	UNP O00481
L	520	SER	-	expression tag	UNP O00481
L	521	HIS	-	expression tag	UNP O00481
L	522	PRO	-	expression tag	UNP O00481

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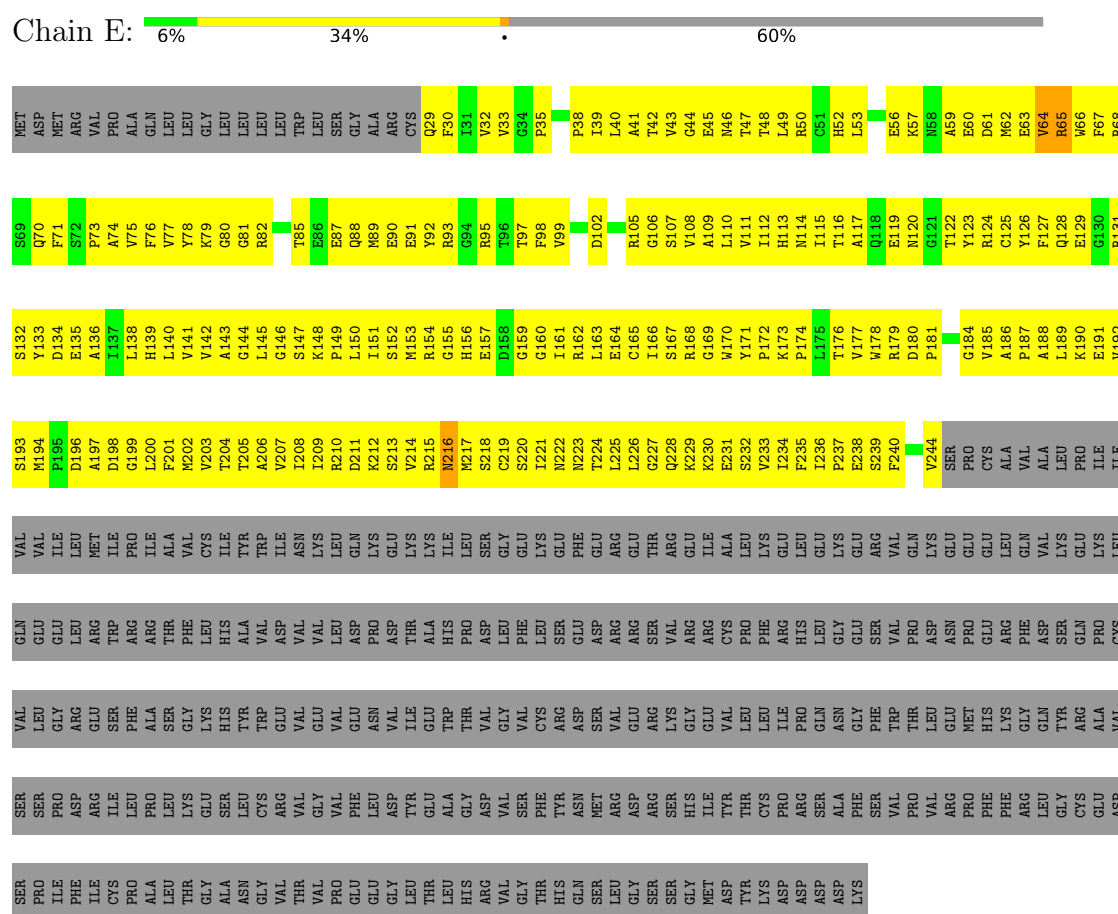
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Chain	Residue	Modelled	Actual	Comment	Reference
L	523	GLN	-	expression tag	UNP O00481
L	524	PHE	-	expression tag	UNP O00481
L	525	GLU	-	expression tag	UNP O00481
L	526	LYS	-	expression tag	UNP O00481
L	527	GLY	-	expression tag	UNP O00481
L	528	GLY	-	expression tag	UNP O00481
L	529	GLY	-	expression tag	UNP O00481
L	530	SER	-	expression tag	UNP O00481
L	531	GLY	-	expression tag	UNP O00481
L	532	GLY	-	expression tag	UNP O00481
L	533	GLY	-	expression tag	UNP O00481
L	534	SER	-	expression tag	UNP O00481
L	535	GLY	-	expression tag	UNP O00481
L	536	GLY	-	expression tag	UNP O00481
L	537	SER	-	expression tag	UNP O00481
L	538	ALA	-	expression tag	UNP O00481
L	539	TRP	-	expression tag	UNP O00481
L	540	SER	-	expression tag	UNP O00481
L	541	HIS	-	expression tag	UNP O00481
L	542	PRO	-	expression tag	UNP O00481
L	543	GLN	-	expression tag	UNP O00481
L	544	PHE	-	expression tag	UNP O00481
L	545	GLU	-	expression tag	UNP O00481
L	546	LYS	-	expression tag	UNP O00481

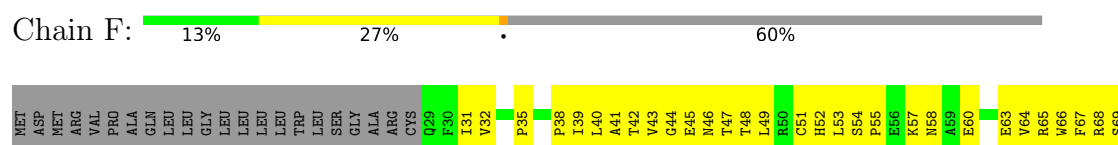
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Butyrophilin subfamily 2 member A1



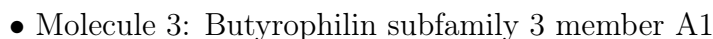
#### • Molecule 1: Butyrophilin subfamily 2 member A1







Digital Tool Type	Percentage
Green	22%
Yellow	41%
Grey	36%



Frequency	Percentage
Very often	14%
Often	23%
Sometimes	17%
Never	60%



Response	Percentage
Current government is the best	12%
Opposition is the best	28%
Neither is the best	60%



LEU	THR	ILE	THR	ASN	GLU	ALA	TTR	G200	K136	S71	MET
THR	ILE	THR	ASN	PHE	SER	TYR	PHE	Y201	A137		ASP
PRO	CYS	ILE	ASN	LEU	ILE	ASN	LEU	Y202	L138	Q74	MET
ALA	PRO	GLY	LEU	TRP	ILE	TRP	GLN	A203	V139	V75	ARG
ALA	LEU	GLY	LYS	TRP	GLY	GLN	GLN	A204	E140	N77	PRO
GLY	PRO	ARG	LYS	LYS	GLY	LYS	GLN	A205	L141		ALA
SER	PRO	ARG	ALA	LYS	ARG	ALA	GLN	A206	K142	V78	ALA
GLY	PRO	HIS	LYS	GLY	HIS	LYS	GLU	S207	V143	Y79	GLN
SER	PRO	TRP	PHE	LEU	GLU	PHE	GLU	V208	A144	D81	LEU
GLY	PRO	TRP	LYS	LYS	LYS	LYS	LYS	I209	A145		LEU
ALA	LYS	GLU	LYS	LYS	G22	LYS	LYS	M210	L146	G82	GLY
TRP	LYS	VAL	PRO	PRO	VAL	PRO	THR		G147	K83	LEU
SER	VAL	GLU	ALA	ALA	GLU	ALA	GLN	V218	S148	E84	LEU
HIS	VAL	VAL	ASP	ASP	PHE	ASP	PHE	S219	D149		LEU
PRO	VAL	VAL	VAL	VAL	ARG	VAL	ARG	L150	E85	E86	LEU
GLY	PHE	ASP	ILE	ILE	ASP	ILE	LYS	T221	H151	D87	TRP
PHE	PHE	LEU	ARG	LEU	ARG	LYS	LYS	I222	V152	R88	LEU
GLY	ASP	LYS	LYS	ASP	LYS	ASP	LYS	R223	D153	Q89	SER
LYS	TYR	GLY	PRO	PRO	ARG	PRO	ARG	S224	V154	S90	GLY
GLY	GLY	TRP	GLY	TRP	TRP	GLY	GLU	S225	K155	A91	ALA
GLY	GLY	GLY	THR	THR	GLU	LYS	GLN	L226	G156	P92	ARG
GLY	GLY	ILE	ALA	ALA	GLY	GLY	GLU	L227	Y157	Y93	ARG
SER	ASP	GLY	ASN	ASN	LEU	ASN	LEU	G228		R94	C29
ILE	VAL	VAL	PRO	PRO	ARG	PRO	ARG	L229	G161	Q30	G30
GLY	GLY	CYS	ILE	ILE	GLU	ILE	GLU	E230	I162	G95	F31
GLY	GLY	SER	LEU	SER	LEU	LEU	MET	T232	H163	R96	S32
SER	TYR	TYR	LEU	LEU	ALA	VAL	ALA	T231		T97	V33
ASN	ASN	ASN	VAL	VAL	SER	VAL	SER	A233	G166	I99	G35
ALA	ALA	VAL	VAL	VAL	SER	GLY	TRP	S234	R167	L100	P36
SER	VAL	GLN	GLU	GLU	GLU	GLU	THR	I235	S168	R101	S37
ALA	ASP	ARG	ARG	ARG	ASP	GLN	MET	S236	T169	D102	G38
TRP	GLY	LYS	GLN	GLN	GLY	ASN	GLY	I237	G170	G103	P39
SER	SER	SER	ARG	ARG	GLY	ARG	GLN	A238	W171	I104	
HIS	HIS	TRP	SER	SER	TRP	SER	GLY	P239	Y172	T105	A42
PRO	PRO	ILE	VAL	VAL	VAL	VAL	GLN	P240	P173	A106	M43
GLN	GLN	LYS	GLN	GLN	LYS	GLN	SER		Q174	G107	V44
PHE	PHE	THR	MET	THR	THR	ARG	THR	S244	P175	K108	G45
GLY	GLY	THR	PRO	ALA	ALA	ALA	ARG	ALA	Q176	A109	E46
LYS	LYS	THR	LYS	LYS	VAL	LYS	VAL	GLN	I177	A110	
	ASP	GLU	GLU	GLU	LYS	GLU	LYS	ARG	L111	R112	L50
	VAL	ASN	PRO	PRO	PRO	PRO	LEU	TRP	W179	I113	C52
	SER	GLY	GLN	GLN	LEU	GLN	LEU	ILE	S180		H53
	PHE	GLY	ASP	ASP	GLY	ASP	LEU	ALA	M181	V116	L54
	PHE	TRP	LEU	LEU	GLU	LEU	GLU	ALA		T117	F55
	LEU	TRP	PRO	PRO	GLY	PRO	LEU	LEU	G184	A118	P56
	LEU	GLY	ASN	ASN	GLY	ASN	TRP	GLY	E185	S119	T57
	LEU	LEU	ASN	ASN	LEU	ASN	ARG	THR	M186	D120	M58
	PRO	THR	PRO	PRO	THR	PRO	ARG	LEU	I187	S121	S59
	VAL	PHE	GLY	GLY	ILE	PHE	ILE	PRO	P188	G122	A60
	ARG	GLY	PHE	GLN	GLN	GLN	GLN	VAL	T189	K123	E81
	ASN	LYS	ASN	TYR	ASN	TYR	ASN	LEU	V190	Y124	T82
	ILE	LYS	TRP	ALA	LEU	TRP	ALA	LEU	E191	L125	M63
	LEU	TYR	HIS	SER	LEU	HIS	SER	LEU	A192		E84
	THR	THR	TYR	ARG	LEU	TYR	ARG	LEU	P193	F128	L65
	ARG	THR	CYS	TYR	GLY	TYR	GLY	LEU	V194	Q129	M67
	GLY	GLY	VAL	VAL	LEU	VAL	GLY	GLY	V195	D130	V68
	THR	THR	LEU	LEU	ARG	LEU	ARG	GLY	A196		S69
	PRO	THR	LEU	LEU	THR	LEU	THR	ALA	D197	Y134	S70
	ALA	THR	CYS	GLY	GLY	GLY	SER	GLY	G198	F135	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229039	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.140	Depositor
Minimum map value	-2.825	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.261	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	517.104, 517.104, 517.104	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3092, 4.3092, 4.3092	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	E	0.35	0/1735	0.63	0/2348
1	F	0.26	0/1735	0.54	0/2348
1	I	0.19	0/1735	0.44	0/2348
1	J	0.25	0/1735	0.53	0/2348
2	G	0.23	0/1663	0.51	2/2255 (0.1%)
2	K	0.26	0/1663	0.59	2/2255 (0.1%)
3	H	0.16	0/1662	0.36	0/2254
3	L	0.25	0/1662	0.49	1/2254 (0.0%)
All	All	0.25	0/13590	0.52	5/18410 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
1	F	0	4
1	J	0	2
3	L	0	1
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	134	TYR	CA-C-N	10.83	141.19	121.70
2	K	134	TYR	C-N-CA	10.83	141.19	121.70
2	G	63	MET	CA-C-N	7.50	135.19	121.70
2	G	63	MET	C-N-CA	7.50	135.19	121.70
3	L	187	ILE	N-CA-C	-5.42	103.00	108.96

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	216	ASN	Peptide
1	E	64	VAL	Peptide
1	E	65	ARG	Peptide
1	F	153	MET	Peptide
1	F	205	THR	Peptide
1	F	60	GLU	Peptide
1	F	72	SER	Peptide
1	J	126	TYR	Peptide
1	J	72	SER	Peptide
3	L	157	TYR	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	E	1698	0	1681	464	0
1	F	1698	0	1681	295	0
1	I	1698	0	1681	189	0
1	J	1698	0	1681	260	0
2	G	1630	0	1596	145	0
2	K	1630	0	1596	179	0
3	H	1629	0	1598	91	0
3	L	1629	0	1598	185	0
All	All	13310	0	13112	1686	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 64.

All (1686) 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:I:154:ARG:NH1	1:I:164:GLU:OE1	1.95	0.99
3:L:37:SER:OG	3:L:137:ALA:O	1.83	0.97
1:E:40:LEU:HD21	1:E:226:LEU:HD23	1.48	0.96
3:L:180:SER:O	3:L:219:SER:OG	1.86	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:164:LEU:HD13	2:K:235:ILE:HG23	1.50	0.91
1:J:65:ARG:NH2	1:J:73:PRO:O	2.03	0.91
1:E:146:GLY:O	1:E:230:LYS:NZ	2.04	0.90
1:E:131:ARG:NH2	3:L:63:MET:SD	2.46	0.89
1:E:97:THR:OG1	1:E:111:VAL:O	1.91	0.89
1:E:41:ALA:HB3	1:E:142:VAL:HG22	1.54	0.87
1:E:173:LYS:NZ	1:E:191:GLU:O	2.07	0.87
1:J:74:ALA:N	1:J:87:GLU:O	2.07	0.87
1:I:32:VAL:HG12	1:I:136:ALA:HB2	1.54	0.86
1:E:119:GLU:O	1:E:123:TYR:OH	1.92	0.86
1:E:85:THR:O	1:E:93:ARG:NH1	2.08	0.86
2:K:118:ALA:HB1	2:K:172:TYR:HB2	1.56	0.86
1:F:190:LYS:NZ	1:F:207:VAL:O	2.09	0.86
1:J:189:LEU:N	1:J:206:ALA:O	2.07	0.86
2:G:219:SER:OG	2:G:233:ALA:O	1.93	0.86
1:E:66:TRP:HB3	1:E:75:VAL:HG23	1.58	0.85
1:F:190:LYS:HG2	1:F:206:ALA:HB1	1.58	0.85
1:F:155:GLY:O	1:F:162:ARG:NH1	2.10	0.85
1:E:106:GLY:O	1:E:108:VAL:HG13	1.75	0.85
1:E:148:LYS:HB3	1:F:150:LEU:HD21	1.59	0.85
1:F:74:ALA:HB3	1:F:77:VAL:HG22	1.59	0.84
1:E:88:GLN:O	1:E:93:ARG:NH2	2.11	0.84
1:F:147:SER:N	1:F:168:ARG:O	2.10	0.84
2:K:57:THR:OG1	2:K:105:THR:O	1.95	0.84
2:K:148:SER:O	2:K:169:THR:N	2.11	0.84
1:I:70:GLN:NE2	1:I:89:MET:SD	2.50	0.83
2:K:192:ALA:HB3	2:K:205:ALA:HB3	1.59	0.83
1:E:32:VAL:HG12	1:E:136:ALA:HB2	1.58	0.83
1:I:150:LEU:N	1:I:166:ILE:O	2.11	0.83
1:J:219:CYS:N	1:J:232:SER:O	2.12	0.83
1:I:214:VAL:HG13	1:I:217:MET:HE2	1.59	0.83
3:L:77:ASN:ND2	3:L:97:THR:O	2.11	0.83
2:G:137:ALA:O	2:G:139:VAL:HG23	1.79	0.82
1:J:47:THR:HG21	1:J:140:LEU:HD22	1.61	0.82
1:J:215:ARG:NH2	1:J:236:ILE:O	2.13	0.82
2:G:54:LEU:HD13	2:G:132:ASP:OD2	1.78	0.82
1:E:117:ALA:N	1:E:119:GLU:OE1	2.13	0.82
1:E:125:CYS:O	1:E:136:ALA:N	2.13	0.81
1:J:127:PHE:N	1:J:128:GLN:OE1	2.10	0.81
1:J:58:ASN:ND2	1:J:129:GLU:OE1	2.13	0.81
1:E:41:ALA:HB2	1:E:140:LEU:HD21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:70:SER:N	2:K:123:LYS:O	2.14	0.81
2:K:178:GLN:OE1	2:K:178:GLN:N	2.13	0.81
1:E:33:VAL:O	1:E:52:HIS:N	2.14	0.80
2:K:177:ILE:HB	2:K:222:ILE:HG23	1.63	0.80
1:E:42:THR:HG22	1:E:43:VAL:H	1.46	0.80
1:E:114:ASN:OD1	1:E:115:ILE:N	2.13	0.80
1:E:124:ARG:NH1	1:E:135:GLU:OE2	2.15	0.80
1:F:151:ILE:HG21	1:F:234:ILE:HB	1.61	0.80
2:G:90:SER:O	2:G:94:ARG:N	2.15	0.80
2:G:197:ASP:OD1	2:G:200:GLY:N	2.15	0.80
1:J:217:MET:HB3	1:J:234:ILE:HG23	1.64	0.80
1:E:153:MET:O	1:E:154:ARG:NE	2.14	0.79
1:E:150:LEU:HD22	1:F:232:SER:HB3	1.65	0.79
3:H:176:GLN:N	3:H:223:ARG:O	2.16	0.79
1:J:219:CYS:O	1:J:232:SER:N	2.16	0.79
1:E:198:ASP:OD1	1:E:199:GLY:N	2.17	0.78
2:G:100:LEU:N	2:G:110:ALA:O	2.17	0.78
2:K:179:TRP:NE1	2:K:206:ALA:HB1	1.99	0.78
1:E:90:GLU:N	1:E:90:GLU:OE1	2.16	0.78
1:I:56:GLU:OE1	1:I:107:SER:OG	2.01	0.78
3:L:118:ALA:HB1	3:L:172:TYR:CD2	2.17	0.78
1:J:228:GLN:OE1	1:J:230:LYS:N	2.17	0.78
3:L:180:SER:HA	3:L:187:ILE:HG22	1.66	0.77
1:E:150:LEU:HD22	1:F:232:SER:CB	2.13	0.77
1:E:231:GLU:OE2	1:F:168:ARG:NH2	2.17	0.77
1:E:74:ALA:O	1:E:89:MET:N	2.16	0.77
1:E:232:SER:HB2	1:F:150:LEU:HD22	1.65	0.77
3:L:171:TRP:O	3:L:202:TYR:N	2.17	0.77
1:J:89:MET:HE1	1:J:116:THR:CG2	2.14	0.77
1:F:235:PHE:O	1:F:236:ILE:HD13	1.84	0.77
3:L:87:ASP:O	3:L:94:ARG:NH1	2.17	0.77
1:E:75:VAL:HG12	1:E:89:MET:HE2	1.65	0.77
1:I:162:ARG:NH2	1:I:164:GLU:OE2	2.18	0.76
1:E:188:ALA:HA	1:E:207:VAL:HG12	1.67	0.76
1:E:88:GLN:NE2	1:E:92:TYR:O	2.18	0.76
1:E:40:LEU:HD11	1:E:143:ALA:HB3	1.65	0.76
2:G:97:THR:OG1	2:G:112:ARG:O	2.01	0.76
2:G:239:ASP:OD1	3:H:157:TYR:OH	2.04	0.75
3:L:44:VAL:HG22	3:L:118:ALA:HB2	1.68	0.75
3:L:82:GLY:O	3:L:101:ARG:NH1	2.20	0.75
1:I:29:GLN:NE2	1:I:129:GLU:OE1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:GLU:N	1:F:157:GLU:OE1	2.20	0.75
1:F:165:CYS:O	1:F:204:THR:OG1	2.02	0.75
1:E:217:MET:O	1:E:234:ILE:HG22	1.85	0.75
1:I:190:LYS:HB2	1:I:206:ALA:HB3	1.69	0.75
1:I:239:SER:OG	1:J:156:HIS:O	2.05	0.75
1:E:53:LEU:HD13	1:E:106:GLY:O	1.87	0.74
1:E:172:PRO:HD2	1:E:225:LEU:HD12	1.68	0.74
1:F:110:LEU:HG	1:F:112:ILE:HD11	1.69	0.74
1:E:152:SER:HA	1:F:234:ILE:HA	1.69	0.74
1:F:165:CYS:N	1:F:205:THR:O	2.21	0.74
3:L:103:GLY:O	3:L:107:GLY:N	2.21	0.74
1:E:40:LEU:HD21	1:E:226:LEU:CD2	2.18	0.74
2:G:172:TYR:O	2:G:224:ASN:ND2	2.20	0.74
2:K:176:GLN:OE1	2:K:225:SER:N	2.19	0.74
1:I:69:SER:O	1:I:124:ARG:NH2	2.20	0.74
2:K:91:ALA:O	2:K:96:ARG:NH2	2.21	0.74
2:K:163:HIS:ND1	2:K:208:VAL:O	2.18	0.74
1:E:91:GLU:OE2	1:E:116:THR:OG1	2.06	0.74
3:H:166:CYS:SG	3:H:206:ALA:HB3	2.28	0.74
2:K:194:VAL:HG12	2:K:204:VAL:HB	1.70	0.74
1:J:91:GLU:OE1	1:J:116:THR:N	2.21	0.73
1:E:190:LYS:HB2	1:E:206:ALA:HB3	1.70	0.73
3:H:179:TRP:NE1	3:H:206:ALA:HB1	2.02	0.73
1:E:198:ASP:OD1	1:E:200:LEU:N	2.22	0.73
3:L:69:SER:N	3:L:74:GLN:O	2.22	0.73
1:F:215:ARG:NH1	1:F:236:ILE:O	2.21	0.73
1:J:172:PRO:O	1:J:193:SER:OG	2.07	0.73
3:H:174:GLN:O	3:H:225:SER:OG	2.04	0.73
1:I:151:ILE:HA	1:I:165:CYS:HA	1.71	0.73
1:E:29:GLN:OE1	1:E:132:SER:OG	2.05	0.73
1:E:152:SER:O	1:E:164:GLU:N	2.20	0.73
1:E:68:ARG:HG3	1:E:123:TYR:CD1	2.23	0.73
1:J:170:TRP:O	1:J:201:PHE:N	2.22	0.73
1:J:53:LEU:HD12	1:J:55:PRO:O	1.89	0.72
2:K:166:CYS:SG	2:K:206:ALA:HB3	2.28	0.72
1:E:239:SER:OG	1:F:157:GLU:O	2.04	0.72
1:E:208:ILE:O	1:E:210:ARG:NH1	2.22	0.72
1:F:215:ARG:O	1:F:236:ILE:N	2.22	0.72
1:J:79:LYS:O	1:J:84:ARG:NH2	2.21	0.72
1:J:163:LEU:N	1:J:207:VAL:O	2.23	0.72
1:I:74:ALA:O	1:I:89:MET:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:42:ALA:HB3	2:K:143:VAL:HG22	1.70	0.72
2:K:69:SER:O	2:K:73:ARG:N	2.23	0.72
1:J:152:SER:O	1:J:164:GLU:N	2.22	0.72
3:L:171:TRP:N	3:L:202:TYR:O	2.22	0.72
1:I:96:THR:HG22	1:I:112:ILE:HA	1.72	0.71
1:E:179:ARG:N	1:E:218:SER:O	2.22	0.71
1:F:65:ARG:NH2	1:F:73:PRO:O	2.23	0.71
1:I:167:SER:OG	1:I:221:ILE:HD12	1.90	0.71
3:H:93:TYR:OH	3:H:117:THR:N	2.21	0.71
1:I:196:ASP:N	1:I:200:LEU:O	2.23	0.71
1:J:128:GLN:OE1	1:J:128:GLN:N	2.22	0.71
3:L:68:VAL:O	3:L:125:LEU:N	2.22	0.71
1:J:174:PRO:CD	1:J:203:VAL:HG21	2.21	0.71
1:E:220:SER:HA	1:E:231:GLU:HA	1.71	0.71
2:G:72:LEU:HD23	2:G:122:GLY:HA2	1.73	0.71
1:E:150:LEU:HD22	1:F:232:SER:HA	1.73	0.71
3:H:122:GLY:O	3:H:141:LEU:HD23	1.90	0.71
1:I:122:THR:OG1	1:I:138:LEU:O	2.05	0.70
3:H:42:ALA:HB3	3:H:141:LEU:CD1	2.21	0.70
1:I:56:GLU:OE2	1:I:107:SER:N	2.22	0.70
1:E:219:CYS:SG	1:E:220:SER:N	2.64	0.70
2:K:171:TRP:CZ2	2:K:222:ILE:HG22	2.26	0.70
1:F:164:GLU:HA	1:F:206:ALA:HA	1.71	0.70
1:I:151:ILE:HD12	1:I:233:VAL:O	1.90	0.70
1:J:61:ASP:OD1	1:J:78:TYR:OH	2.09	0.70
2:K:76:VAL:HG21	2:K:124:TYR:HE2	1.56	0.70
1:E:232:SER:CB	1:F:150:LEU:HD22	2.21	0.69
2:G:164:LEU:HD22	2:G:235:ILE:HG21	1.75	0.69
3:L:65:LEU:HD11	3:L:104:ILE:HD12	1.75	0.69
1:F:66:TRP:NE1	1:F:126:TYR:O	2.26	0.69
1:J:174:PRO:CG	1:J:203:VAL:HG21	2.23	0.69
2:K:169:THR:HG22	2:K:203:GLU:HB3	1.73	0.69
3:L:62:THR:HG23	3:L:63:MET:HG2	1.75	0.69
1:I:144:GLY:N	1:I:171:TYR:O	2.26	0.69
1:E:152:SER:OG	1:F:235:PHE:N	2.26	0.69
1:F:65:ARG:NH2	1:F:74:ALA:HB2	2.07	0.69
1:F:116:THR:HG23	1:F:119:GLU:H	1.58	0.69
3:L:29:CYS:N	3:L:130:ASP:O	2.26	0.69
1:E:190:LYS:O	1:E:206:ALA:N	2.25	0.69
3:H:42:ALA:HB3	3:H:141:LEU:HD13	1.75	0.69
1:F:222:ASN:O	1:F:223:ASN:ND2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:PRO:HD2	1:J:214:VAL:HG12	1.74	0.68
1:I:75:VAL:HG22	1:I:89:MET:HE2	1.75	0.68
3:L:86:GLU:OE1	3:L:86:GLU:N	2.26	0.68
1:J:221:ILE:O	1:J:228:GLN:NE2	2.26	0.68
2:K:224:ASN:N	2:K:229:LEU:O	2.24	0.68
1:E:196:ASP:O	1:E:199:GLY:N	2.27	0.68
2:K:76:VAL:HG22	2:K:93:TYR:CD2	2.29	0.68
3:L:67:TRP:HB2	3:L:99:ILE:HD11	1.76	0.68
1:E:53:LEU:HD11	1:E:127:PHE:CD2	2.28	0.68
1:I:232:SER:HA	1:J:150:LEU:HD22	1.74	0.68
1:J:217:MET:N	1:J:234:ILE:O	2.27	0.68
1:J:151:ILE:HD13	1:J:234:ILE:HG22	1.74	0.67
1:E:117:ALA:HA	1:E:142:VAL:HG21	1.77	0.67
1:J:150:LEU:HD12	1:J:151:ILE:N	2.08	0.67
1:E:148:LYS:HA	1:E:230:LYS:HB3	1.77	0.67
2:K:148:SER:N	2:K:169:THR:O	2.26	0.67
3:L:67:TRP:CE3	3:L:111:LEU:HD22	2.30	0.67
3:L:76:VAL:O	3:L:97:THR:OG1	2.12	0.67
1:E:221:ILE:N	1:E:230:LYS:O	2.27	0.67
2:G:67:TRP:CH2	2:G:99:ILE:HG21	2.29	0.67
1:E:172:PRO:CD	1:E:225:LEU:HD12	2.24	0.67
1:E:95:ARG:NH2	1:E:119:GLU:OE2	2.28	0.67
1:F:49:LEU:O	1:F:110:LEU:N	2.28	0.67
1:I:150:LEU:HD22	1:J:232:SER:HA	1.76	0.67
1:E:157:GLU:O	1:E:160:GLY:N	2.27	0.66
2:G:146:LEU:HD22	2:G:229:LEU:HD12	1.77	0.66
3:H:120:ASP:O	3:H:124:TYR:OH	2.11	0.66
1:E:43:VAL:HG22	1:E:200:LEU:HD21	1.76	0.66
1:E:176:THR:OG1	1:E:191:GLU:OE2	2.13	0.66
1:J:131:ARG:NH1	2:K:66:LYS:O	2.28	0.66
3:L:50:LEU:HD21	3:L:141:LEU:HD21	1.77	0.66
3:L:192:ALA:HB3	3:L:205:ALA:HB1	1.77	0.66
1:I:43:VAL:HG23	1:I:144:GLY:HA2	1.77	0.66
1:I:231:GLU:OE1	1:J:168:ARG:NH1	2.27	0.66
1:I:124:ARG:NH1	1:I:135:GLU:OE1	2.29	0.66
1:I:147:SER:OG	1:I:150:LEU:HD21	1.95	0.66
1:E:177:VAL:HG23	1:E:220:SER:HB2	1.78	0.66
1:E:149:PRO:HG3	1:E:221:ILE:H	1.59	0.66
1:F:212:LYS:O	1:F:215:ARG:NH2	2.28	0.66
1:J:41:ALA:HB3	1:J:115:ILE:HB	1.76	0.66
1:I:90:GLU:OE1	1:I:90:GLU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:41:LEU:HD21	2:K:227:LEU:HD21	1.77	0.66
1:F:45:GLU:O	1:F:114:ASN:N	2.29	0.66
1:E:234:ILE:HG23	1:E:234:ILE:O	1.95	0.66
1:I:150:LEU:HD22	1:J:232:SER:HB3	1.76	0.66
1:E:95:ARG:HH22	1:E:116:THR:HG23	1.59	0.65
1:E:97:THR:OG1	1:E:113:HIS:NE2	2.28	0.65
1:E:151:ILE:HA	1:E:165:CYS:HA	1.77	0.65
1:I:158:ASP:O	1:I:210:ARG:NH1	2.29	0.65
1:J:173:LYS:O	1:J:224:THR:HG23	1.95	0.65
1:E:174:PRO:O	1:E:203:VAL:HG11	1.95	0.65
1:E:234:ILE:HA	1:F:152:SER:HA	1.79	0.65
2:K:197:ASP:OD1	2:K:201:LEU:N	2.29	0.65
1:F:65:ARG:HH22	1:F:74:ALA:HB2	1.61	0.65
1:I:41:ALA:N	1:I:141:VAL:O	2.29	0.65
1:I:59:ALA:HB1	1:I:64:VAL:HG21	1.79	0.65
2:K:76:VAL:HG21	2:K:124:TYR:CE2	2.32	0.65
2:K:177:ILE:HG21	2:K:204:VAL:HG21	1.79	0.65
1:J:67:PHE:HA	1:J:75:VAL:HG22	1.77	0.65
1:J:158:ASP:O	1:J:210:ARG:NE	2.30	0.65
3:L:186:ASN:ND2	3:L:230:GLU:OE2	2.29	0.65
1:E:56:GLU:OE2	1:E:107:SER:OG	2.05	0.65
1:J:153:MET:HA	1:J:162:ARG:O	1.97	0.65
3:L:103:GLY:O	3:L:106:ALA:N	2.30	0.65
1:E:39:ILE:HG22	1:E:47:THR:HG22	1.80	0.65
1:J:126:TYR:OH	1:J:135:GLU:OE2	2.14	0.65
2:K:50:LEU:HD22	2:K:124:TYR:CE1	2.32	0.65
3:L:32:SER:O	3:L:55:PHE:N	2.29	0.64
1:E:116:THR:N	1:E:119:GLU:OE2	2.28	0.64
3:H:176:GLN:O	3:H:223:ARG:N	2.26	0.64
1:E:41:ALA:CB	1:E:142:VAL:HG22	2.26	0.64
1:I:67:PHE:HA	1:I:75:VAL:HG23	1.78	0.64
1:J:210:ARG:NH1	1:J:210:ARG:O	2.30	0.64
1:F:47:THR:CG2	1:F:140:LEU:HD13	2.27	0.64
1:I:77:VAL:HG21	1:I:87:GLU:HG3	1.80	0.64
3:L:77:ASN:OD1	3:L:78:VAL:N	2.30	0.64
1:E:70:GLN:O	1:E:74:ALA:HB2	1.98	0.64
1:F:39:ILE:O	1:F:140:LEU:HD11	1.98	0.64
1:F:178:TRP:CD1	1:F:205:THR:HG22	2.33	0.64
1:F:190:LYS:CG	1:F:206:ALA:HB1	2.26	0.64
1:J:40:LEU:HB3	1:J:143:ALA:HB2	1.80	0.64
1:F:42:THR:OG1	1:F:143:ALA:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:VAL:HG23	3:H:135:GLU:OE2	1.97	0.64
1:E:236:ILE:HG23	1:E:237:PRO:HD2	1.80	0.64
1:J:43:VAL:HB	1:J:200:LEU:HD11	1.80	0.64
2:K:76:VAL:HG22	2:K:93:TYR:CE2	2.33	0.64
1:I:43:VAL:HG22	1:I:200:LEU:CD2	2.28	0.64
1:I:95:ARG:O	1:I:113:HIS:N	2.28	0.64
1:J:53:LEU:HD13	1:J:57:LYS:HE2	1.78	0.64
1:J:114:ASN:O	1:J:115:ILE:HD13	1.97	0.64
1:I:157:GLU:N	1:I:160:GLY:O	2.25	0.64
1:E:234:ILE:HG12	1:F:153:MET:SD	2.38	0.64
1:F:95:ARG:O	1:F:113:HIS:N	2.30	0.64
1:I:65:ARG:NH2	1:I:77:VAL:HG22	2.13	0.63
1:I:116:THR:HG23	1:I:117:ALA:H	1.62	0.63
2:K:192:ALA:HB3	2:K:205:ALA:CB	2.28	0.63
1:J:157:GLU:OE2	1:J:162:ARG:N	2.31	0.63
1:J:89:MET:HE1	1:J:116:THR:HG21	1.80	0.63
1:E:214:VAL:O	1:E:215:ARG:NH2	2.32	0.63
2:K:74:GLN:O	2:K:76:VAL:HG23	1.99	0.63
3:L:50:LEU:HD22	3:L:139:VAL:CG1	2.29	0.63
1:E:43:VAL:HG22	1:E:200:LEU:CD2	2.29	0.63
3:L:224:SER:O	3:L:228:GLY:N	2.30	0.63
1:F:49:LEU:N	1:F:110:LEU:O	2.31	0.63
2:G:177:ILE:O	2:G:189:ALA:N	2.27	0.63
1:I:43:VAL:HG22	1:I:200:LEU:HD22	1.80	0.63
2:K:47:ASP:OD1	2:K:116:VAL:N	2.30	0.63
2:K:77:ASN:ND2	2:K:97:THR:O	2.32	0.63
1:E:39:ILE:HD12	1:E:138:LEU:HD21	1.79	0.63
3:H:148:SER:OG	3:H:169:THR:N	2.30	0.63
1:E:148:LYS:CB	1:F:150:LEU:HD21	2.28	0.62
1:E:153:MET:HA	1:E:162:ARG:O	1.98	0.62
3:H:169:THR:HB	3:H:195:VAL:HG23	1.80	0.62
1:J:149:PRO:HB2	1:J:232:SER:HB3	1.81	0.62
1:J:214:VAL:HG23	1:J:236:ILE:HB	1.81	0.62
2:K:154:VAL:HG22	2:K:164:LEU:HD23	1.81	0.62
1:E:163:LEU:O	1:E:207:VAL:N	2.28	0.62
1:F:151:ILE:HD11	1:F:232:SER:O	1.99	0.62
3:L:68:VAL:HB	3:L:125:LEU:HD12	1.79	0.62
1:E:178:TRP:NE1	1:E:205:THR:HG21	2.15	0.62
1:E:216:ASN:HA	1:E:235:PHE:HA	1.82	0.62
1:F:74:ALA:HB3	1:F:77:VAL:CG2	2.28	0.62
1:F:155:GLY:O	1:F:162:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:ILE:HD13	1:F:204:THR:HB	1.81	0.62
1:F:175:LEU:HD13	1:F:223:ASN:HA	1.81	0.62
2:G:192:ALA:HB3	2:G:205:ALA:N	2.14	0.62
1:I:151:ILE:HD12	1:J:151:ILE:O	1.99	0.62
1:J:48:THR:HA	1:J:111:VAL:HG22	1.80	0.62
1:J:165:CYS:SG	1:J:232:SER:OG	2.55	0.62
2:G:192:ALA:HB1	2:G:193:PRO:HD2	1.79	0.62
1:I:47:THR:HG21	1:I:140:LEU:HD11	1.81	0.62
1:E:41:ALA:HB2	1:E:140:LEU:CD2	2.28	0.62
1:E:57:LYS:NZ	1:E:128:GLN:O	2.32	0.62
2:G:178:GLN:HA	2:G:189:ALA:HB3	1.81	0.62
3:L:171:TRP:CD1	3:L:204:VAL:HG22	2.34	0.62
1:F:218:SER:HA	1:F:233:VAL:HA	1.81	0.62
3:H:50:LEU:HD13	3:H:124:TYR:HB2	1.81	0.62
1:E:95:ARG:NH2	1:E:116:THR:HG23	2.15	0.62
1:E:150:LEU:HD22	1:F:232:SER:CA	2.29	0.62
2:K:208:VAL:HG21	2:K:218:VAL:HG11	1.81	0.62
3:L:65:LEU:O	3:L:99:ILE:HD13	2.00	0.62
1:E:186:ALA:N	1:E:217:MET:SD	2.72	0.62
1:F:91:GLU:OE1	1:F:116:THR:HG22	2.00	0.62
1:F:161:ILE:O	1:F:209:ILE:N	2.32	0.62
2:G:70:SER:OG	2:G:125:LEU:N	2.32	0.62
2:G:235:ILE:HD12	3:H:152:VAL:HG21	1.80	0.62
1:I:150:LEU:HD23	1:J:150:LEU:HA	1.81	0.62
1:E:79:LYS:HB2	3:L:134:TYR:CZ	2.35	0.62
1:E:151:ILE:HD12	1:E:234:ILE:HB	1.82	0.61
1:J:47:THR:HG21	1:J:140:LEU:CD2	2.30	0.61
2:K:49:ASP:OD1	2:K:50:LEU:N	2.34	0.61
3:H:176:GLN:O	3:H:178:GLN:NE2	2.33	0.61
1:J:97:THR:OG1	1:J:111:VAL:O	2.15	0.61
1:F:47:THR:HG21	1:F:140:LEU:HD13	1.82	0.61
1:E:187:PRO:O	1:E:210:ARG:NH1	2.33	0.61
1:J:32:VAL:HG21	1:J:136:ALA:HB1	1.81	0.61
2:K:72:LEU:HD13	2:K:119:SER:O	2.00	0.61
1:F:189:LEU:H	1:F:206:ALA:HB3	1.64	0.61
1:I:223:ASN:OD1	1:I:226:LEU:N	2.32	0.61
1:J:150:LEU:HD11	1:J:166:ILE:HD13	1.83	0.61
2:G:65:LEU:O	2:G:65:LEU:HD23	2.01	0.61
2:K:76:VAL:O	2:K:97:THR:OG1	2.15	0.61
1:I:65:ARG:NE	1:I:71:PHE:O	2.30	0.61
1:E:149:PRO:HB3	1:E:165:CYS:SG	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:THR:OG1	3:L:119:SER:OG	2.19	0.61
1:E:41:ALA:HB1	1:E:115:ILE:HG13	1.83	0.61
2:G:69:SER:OG	2:G:74:GLN:NE2	2.34	0.61
2:K:50:LEU:HD13	2:K:124:TYR:CZ	2.36	0.61
1:E:91:GLU:O	1:E:95:ARG:NH2	2.30	0.60
2:G:37:SER:HA	2:G:139:VAL:HG22	1.83	0.60
2:G:176:GLN:O	2:G:223:ARG:N	2.33	0.60
1:J:39:ILE:HB	1:J:47:THR:HG23	1.83	0.60
1:F:217:MET:HB3	1:F:234:ILE:HG23	1.83	0.60
1:F:163:LEU:N	1:F:207:VAL:O	2.35	0.60
2:K:230:GLU:OE1	2:K:230:GLU:N	2.33	0.60
2:G:146:LEU:HD12	2:G:171:TRP:CZ3	2.37	0.60
3:L:192:ALA:HB1	3:L:193:PRO:HD2	1.82	0.60
1:E:52:HIS:O	1:E:53:LEU:HD12	2.02	0.60
1:E:65:ARG:NH2	1:E:87:GLU:OE2	2.20	0.60
1:F:63:GLU:O	1:F:64:VAL:HG23	2.01	0.60
2:K:113:ILE:HD11	2:K:124:TYR:OH	2.00	0.60
1:E:49:LEU:HD12	1:E:138:LEU:HD22	1.82	0.60
2:G:153:GLU:OE1	2:G:163:HIS:ND1	2.34	0.60
3:H:192:ALA:HB1	3:H:193:PRO:HD2	1.83	0.60
1:E:230:LYS:HZ1	1:F:148:LYS:HG3	1.67	0.60
1:F:151:ILE:HG21	1:F:234:ILE:CB	2.31	0.60
3:H:42:ALA:HB1	3:H:46:GLU:OE1	2.02	0.60
3:H:48:ALA:HB1	3:H:141:LEU:HD22	1.82	0.60
1:I:47:THR:CB	1:I:140:LEU:HD11	2.31	0.60
3:L:65:LEU:HD11	3:L:104:ILE:CD1	2.31	0.60
3:L:194:VAL:HG12	3:L:204:VAL:HA	1.83	0.60
1:E:65:ARG:HD2	1:E:71:PHE:HA	1.84	0.59
1:F:152:SER:N	1:F:164:GLU:O	2.32	0.59
1:E:66:TRP:O	1:E:74:ALA:HB1	2.02	0.59
1:I:59:ALA:HB1	1:I:64:VAL:CG2	2.32	0.59
1:E:216:ASN:O	1:E:236:ILE:HD12	2.02	0.59
1:I:150:LEU:HD22	1:J:232:SER:CB	2.33	0.59
1:E:39:ILE:HD13	1:E:48:THR:O	2.02	0.59
1:F:31:ILE:HD12	1:F:134:ASP:OD1	2.02	0.59
1:I:92:TYR:HB3	1:I:96:THR:HG23	1.83	0.59
1:I:155:GLY:O	1:I:162:ARG:N	2.35	0.59
3:L:50:LEU:HD21	3:L:141:LEU:CD2	2.33	0.59
1:F:39:ILE:HD12	1:F:48:THR:H	1.68	0.59
1:I:66:TRP:O	1:I:75:VAL:N	2.32	0.59
1:E:153:MET:O	1:F:235:PHE:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ARG:N	1:E:162:ARG:O	2.35	0.59
1:J:120:ASN:OD1	1:J:141:VAL:HG13	2.03	0.59
1:J:176:THR:HA	1:J:221:ILE:HA	1.84	0.59
3:H:50:LEU:HD11	3:H:113:ILE:HD11	1.84	0.59
1:F:167:SER:OG	1:F:221:ILE:HD11	2.03	0.58
2:G:43:MET:SD	2:G:144:ALA:HB3	2.43	0.58
1:J:151:ILE:HG23	1:J:164:GLU:O	2.02	0.58
2:K:144:ALA:HB2	2:K:226:LEU:HD23	1.84	0.58
1:E:39:ILE:HG21	1:E:48:THR:OG1	2.03	0.58
2:G:164:LEU:HD13	2:G:235:ILE:HG23	1.85	0.58
3:H:50:LEU:HD11	3:H:113:ILE:CD1	2.33	0.58
1:J:60:GLU:O	1:J:78:TYR:OH	2.16	0.58
2:K:133:PHE:C	2:K:135:GLU:HA	2.29	0.58
3:L:50:LEU:HD13	3:L:139:VAL:HG11	1.84	0.58
1:E:66:TRP:CZ2	1:E:108:VAL:HG21	2.38	0.58
1:F:46:ASN:ND2	1:F:111:VAL:HG12	2.19	0.58
1:F:165:CYS:N	1:F:178:TRP:CZ2	2.72	0.58
1:J:32:VAL:CG2	1:J:136:ALA:HB1	2.33	0.58
3:L:195:VAL:O	3:L:203:ALA:N	2.37	0.58
3:L:154:VAL:HG22	3:L:155:LYS:H	1.69	0.58
1:E:234:ILE:HG13	1:F:152:SER:HA	1.85	0.58
1:I:49:LEU:HD23	1:I:66:TRP:HB3	1.85	0.58
1:I:157:GLU:OE1	1:I:208:ILE:HG23	2.03	0.58
2:K:124:TYR:O	2:K:139:VAL:N	2.37	0.58
3:H:33:VAL:HG22	3:H:54:LEU:HG	1.85	0.58
2:K:33:VAL:HG13	2:K:51:PRO:O	2.04	0.58
1:E:52:HIS:C	1:E:53:LEU:HD12	2.28	0.58
1:E:97:THR:N	1:E:111:VAL:O	2.36	0.58
1:E:150:LEU:HB2	1:E:166:ILE:HB	1.86	0.58
1:E:179:ARG:O	1:E:218:SER:N	2.36	0.58
1:F:180:ASP:HB3	1:F:217:MET:SD	2.44	0.58
1:J:186:ALA:HB1	1:J:207:VAL:HG21	1.86	0.58
1:E:178:TRP:HE1	1:E:205:THR:HG21	1.69	0.58
1:F:150:LEU:O	1:F:151:ILE:HD13	2.02	0.58
2:G:221:ILE:CD1	2:G:232:THR:HG23	2.33	0.58
3:L:171:TRP:CE3	3:L:175:PRO:HG3	2.38	0.58
3:H:175:PRO:HG2	3:H:204:VAL:HG11	1.86	0.57
3:L:31:PHE:HB3	3:L:58:MET:HE2	1.85	0.57
1:E:178:TRP:HB2	1:E:185:VAL:HG13	1.85	0.57
1:F:150:LEU:HB2	1:F:166:ILE:C	2.29	0.57
2:G:97:THR:OG1	2:G:113:ILE:HD13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:THR:HG22	1:I:43:VAL:H	1.69	0.57
1:J:53:LEU:HD22	1:J:128:GLN:CB	2.34	0.57
1:J:91:GLU:OE2	1:J:116:THR:HB	2.03	0.57
2:K:78:VAL:HG21	2:K:88:ARG:NE	2.18	0.57
2:K:90:SER:O	2:K:94:ARG:N	2.37	0.57
2:K:167:ARG:HA	2:K:205:ALA:HA	1.86	0.57
3:L:97:THR:HB	3:L:111:LEU:HD11	1.86	0.57
3:L:118:ALA:HB1	3:L:172:TYR:CE2	2.38	0.57
1:E:65:ARG:NH1	1:E:77:VAL:HG21	2.18	0.57
2:G:54:LEU:HD11	2:G:126:CYS:HB2	1.87	0.57
2:K:45:GLY:N	2:K:116:VAL:O	2.37	0.57
2:K:71:SER:OG	2:K:121:SER:O	2.15	0.57
1:E:43:VAL:HA	1:E:200:LEU:HD22	1.85	0.57
1:E:125:CYS:N	1:E:136:ALA:HB3	2.18	0.57
3:H:149:ASP:C	3:H:150:LEU:HD22	2.29	0.57
1:E:151:ILE:HD11	1:E:232:SER:HB3	1.86	0.57
1:I:186:ALA:HB3	1:I:207:VAL:HG11	1.86	0.57
2:K:177:ILE:HA	2:K:222:ILE:HA	1.87	0.57
2:K:208:VAL:HG11	2:K:218:VAL:CG1	2.34	0.57
1:E:56:GLU:OE2	1:E:105:ARG:NH2	2.38	0.57
1:E:123:TYR:CE2	1:E:140:LEU:HB3	2.40	0.57
1:F:42:THR:HG22	1:F:43:VAL:N	2.20	0.57
2:G:172:TYR:OH	2:G:200:GLY:O	2.20	0.57
2:G:55:PHE:HA	2:G:106:ALA:HB1	1.86	0.57
2:G:220:CYS:O	2:G:221:ILE:HD13	2.05	0.57
2:G:224:ASN:O	2:G:228:GLY:N	2.37	0.57
1:I:235:PHE:HB3	1:J:154:ARG:CZ	2.35	0.57
1:E:47:THR:HG21	1:E:140:LEU:HD21	1.86	0.57
2:G:116:VAL:HG21	2:G:141:LEU:HD11	1.87	0.57
3:L:118:ALA:HA	3:L:143:VAL:HG12	1.86	0.57
3:L:168:SER:OG	3:L:171:TRP:NE1	2.28	0.57
2:G:77:ASN:OD1	2:G:78:VAL:N	2.38	0.57
2:G:171:TRP:CE3	2:G:224:ASN:HB2	2.40	0.57
2:G:176:GLN:N	2:G:223:ARG:O	2.28	0.57
3:L:187:ILE:HG13	3:L:188:PRO:HD2	1.86	0.57
1:I:32:VAL:HG12	1:I:136:ALA:CB	2.30	0.57
1:J:164:GLU:HA	1:J:206:ALA:HA	1.87	0.57
1:E:41:ALA:HB3	1:E:142:VAL:HA	1.87	0.56
1:E:164:GLU:HB2	1:E:205:THR:O	2.05	0.56
3:H:116:VAL:O	3:H:116:VAL:HG13	2.05	0.56
3:H:194:VAL:HB	3:H:203:ALA:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ARG:CZ	1:E:206:ALA:HB1	2.36	0.56
2:G:176:GLN:OE1	2:G:225:SER:N	2.37	0.56
1:J:196:ASP:O	1:J:199:GLY:N	2.37	0.56
1:E:53:LEU:HD11	1:E:127:PHE:CE2	2.41	0.56
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.56
1:E:234:ILE:HA	1:F:152:SER:CB	2.35	0.56
2:K:167:ARG:NH1	2:K:203:GLU:O	2.37	0.56
3:L:97:THR:HG22	3:L:113:ILE:HA	1.86	0.56
1:F:163:LEU:O	1:F:207:VAL:N	2.38	0.56
1:F:180:ASP:HB2	1:F:214:VAL:HG21	1.87	0.56
1:I:59:ALA:HB3	1:I:103:ILE:O	2.05	0.56
1:I:156:HIS:HB2	1:J:239:SER:OG	2.05	0.56
3:L:178:GLN:N	3:L:221:THR:O	2.29	0.56
1:E:149:PRO:HD3	1:E:230:LYS:C	2.31	0.56
1:I:121:GLY:O	1:I:140:LEU:N	2.36	0.56
1:J:219:CYS:O	1:J:232:SER:OG	2.23	0.56
3:L:150:LEU:HD22	3:L:166:CYS:HB2	1.86	0.56
1:I:177:VAL:HG12	1:I:220:SER:O	2.04	0.56
1:J:77:VAL:HG21	1:J:87:GLU:HB2	1.87	0.56
1:E:171:TYR:C	1:E:174:PRO:HD3	2.31	0.56
1:F:155:GLY:N	1:F:162:ARG:O	2.31	0.56
1:E:59:ALA:HB1	1:E:62:MET:HB2	1.88	0.56
1:F:152:SER:CB	1:F:164:GLU:HG3	2.36	0.56
1:J:42:THR:HG22	1:J:43:VAL:H	1.71	0.56
1:J:179:ARG:N	1:J:218:SER:O	2.38	0.55
1:J:194:MET:O	1:J:194:MET:SD	2.63	0.55
1:E:147:SER:OG	1:E:148:LYS:N	2.40	0.55
1:E:168:ARG:H	1:E:168:ARG:HD3	1.72	0.55
3:H:116:VAL:HG21	3:H:141:LEU:HD21	1.87	0.55
1:J:187:PRO:O	1:J:207:VAL:HG23	2.05	0.55
1:E:233:VAL:HG21	1:E:235:PHE:HE1	1.72	0.55
3:L:34:LEU:N	3:L:53:HIS:O	2.40	0.55
3:L:189:THR:HG21	3:L:191:GLU:HG3	1.88	0.55
2:G:186:ASN:OD1	2:G:223:ARG:HD2	2.06	0.55
1:F:163:LEU:HD23	1:F:234:ILE:HG21	1.88	0.55
1:I:180:ASP:OD1	1:I:217:MET:SD	2.64	0.55
2:K:122:GLY:N	2:K:141:LEU:O	2.40	0.55
2:K:148:SER:OG	2:K:169:THR:OG1	2.23	0.55
2:K:236:SER:OG	2:K:237:ILE:N	2.35	0.55
1:E:74:ALA:O	1:E:88:GLN:HA	2.06	0.55
1:F:35:PRO:CG	1:F:49:LEU:HD23	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ARG:O	1:F:218:SER:HB3	2.07	0.55
1:J:53:LEU:HD22	1:J:128:GLN:HB2	1.88	0.55
1:E:48:THR:HA	1:E:111:VAL:HG13	1.89	0.55
1:E:70:GLN:NE2	1:E:89:MET:SD	2.79	0.55
3:H:191:GLU:OE2	3:H:204:VAL:HG12	2.06	0.55
1:I:47:THR:CG2	1:I:140:LEU:HD11	2.36	0.55
2:K:116:VAL:HG13	2:K:120:ASP:HB2	1.89	0.55
1:E:164:GLU:O	1:E:164:GLU:HG2	2.06	0.55
1:E:177:VAL:N	1:E:220:SER:O	2.31	0.55
1:E:177:VAL:HG21	1:E:229:LYS:HE3	1.89	0.55
1:F:150:LEU:CB	1:F:166:ILE:HB	2.36	0.55
2:G:116:VAL:CG2	2:G:141:LEU:HD11	2.37	0.55
1:J:174:PRO:HG3	1:J:203:VAL:HG21	1.88	0.55
3:L:69:SER:O	3:L:71:SER:N	2.38	0.55
1:E:235:PHE:HB3	1:F:154:ARG:HD2	1.89	0.55
3:H:221:THR:HG22	3:H:232:THR:HG23	1.88	0.55
1:I:59:ALA:HB2	1:I:106:GLY:HA2	1.88	0.55
1:I:233:VAL:O	1:J:152:SER:HB2	2.06	0.55
1:J:68:ARG:O	1:J:124:ARG:HG2	2.06	0.55
1:J:89:MET:HG2	1:J:90:GLU:N	2.21	0.55
1:J:175:LEU:N	1:J:222:ASN:O	2.40	0.54
3:L:50:LEU:HD22	3:L:139:VAL:HG13	1.89	0.54
3:L:70:SER:N	3:L:123:LYS:O	2.37	0.54
1:E:153:MET:CA	1:E:162:ARG:O	2.55	0.54
2:G:164:LEU:HD22	2:G:235:ILE:CG2	2.36	0.54
2:G:224:ASN:OD1	2:G:225:SER:N	2.40	0.54
1:I:151:ILE:HG21	1:I:234:ILE:HD12	1.89	0.54
1:J:219:CYS:HB3	1:J:232:SER:OG	2.07	0.54
2:K:169:THR:HA	2:K:203:GLU:HA	1.88	0.54
1:E:152:SER:N	1:E:164:GLU:O	2.35	0.54
3:H:179:TRP:CD1	3:H:189:THR:HG1	2.25	0.54
1:E:64:VAL:CG2	1:E:127:PHE:HA	2.37	0.54
1:I:30:PHE:CE1	1:I:53:LEU:HD22	2.43	0.54
1:I:47:THR:HB	1:I:140:LEU:HD11	1.90	0.54
1:I:234:ILE:HG13	1:J:153:MET:SD	2.48	0.54
1:J:66:TRP:N	1:J:76:PHE:O	2.34	0.54
1:J:152:SER:HB3	1:J:164:GLU:HB2	1.88	0.54
2:K:116:VAL:HG13	2:K:120:ASP:CB	2.38	0.54
1:F:187:PRO:HD2	1:F:207:VAL:HG23	1.90	0.54
3:L:180:SER:CA	3:L:187:ILE:HG22	2.37	0.54
2:G:222:ILE:HG22	2:G:223:ARG:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:41:LEU:HD12	3:H:142:LYS:HE3	1.89	0.54
1:I:129:GLU:OE1	1:I:129:GLU:N	2.41	0.54
1:I:151:ILE:HD13	1:I:234:ILE:HB	1.88	0.54
1:E:170:TRP:HB3	1:E:174:PRO:HG2	1.90	0.54
1:F:160:GLY:O	1:F:161:ILE:HG23	2.07	0.54
1:I:65:ARG:HH22	1:I:77:VAL:HG22	1.71	0.54
1:J:163:LEU:O	1:J:206:ALA:HA	2.08	0.54
2:K:192:ALA:CB	2:K:205:ALA:HB3	2.36	0.54
1:E:170:TRP:HB2	1:E:203:VAL:N	2.22	0.54
1:E:186:ALA:HB3	1:E:207:VAL:HG21	1.90	0.54
1:F:194:MET:SD	1:F:194:MET:O	2.66	0.54
3:L:52:CYS:SG	3:L:67:TRP:CZ2	3.01	0.54
1:E:152:SER:CA	1:F:234:ILE:HA	2.37	0.54
2:G:180:SER:OG	2:G:183:LYS:NZ	2.28	0.54
3:L:192:ALA:HB3	3:L:205:ALA:CB	2.37	0.54
1:F:32:VAL:HG23	1:F:134:ASP:OD2	2.08	0.54
1:F:147:SER:OG	1:F:148:LYS:N	2.39	0.54
1:I:162:ARG:HE	1:I:206:ALA:HB1	1.72	0.54
1:E:180:ASP:OD1	1:E:181:PRO:CD	2.56	0.53
1:I:116:THR:HG23	1:I:117:ALA:N	2.23	0.53
1:I:176:THR:HG23	1:I:221:ILE:HG13	1.90	0.53
1:J:33:VAL:O	1:J:50:ARG:NH1	2.40	0.53
2:K:145:ALA:N	2:K:172:TYR:O	2.32	0.53
3:L:117:THR:O	3:L:120:ASP:N	2.39	0.53
1:E:119:GLU:C	1:E:123:TYR:HH	2.05	0.53
1:F:131:ARG:O	2:G:62:THR:HG21	2.08	0.53
1:J:153:MET:HA	1:J:164:GLU:HG3	1.90	0.53
1:F:162:ARG:HG3	1:F:190:LYS:HE2	1.91	0.53
3:H:44:VAL:HG13	3:H:117:THR:HA	1.89	0.53
1:I:90:GLU:OE2	1:I:93:ARG:NH2	2.39	0.53
1:E:163:LEU:HB2	1:E:207:VAL:HG23	1.91	0.53
1:F:153:MET:HA	1:F:163:LEU:HA	1.91	0.53
1:I:217:MET:O	1:I:234:ILE:HG22	2.08	0.53
1:J:46:ASN:HA	1:J:112:ILE:O	2.08	0.53
1:E:66:TRP:HH2	1:E:78:TYR:CE2	2.26	0.53
1:E:112:ILE:HG22	1:E:113:HIS:N	2.24	0.53
1:E:149:PRO:N	1:F:150:LEU:HD21	2.23	0.53
1:I:150:LEU:HD22	1:J:232:SER:CA	2.38	0.53
1:E:147:SER:HB3	1:E:167:SER:HA	1.91	0.53
1:F:170:TRP:CZ2	1:F:221:ILE:HG21	2.43	0.53
1:F:189:LEU:HD11	1:F:208:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:GLU:OE1	2:G:61:GLU:N	2.42	0.53
2:G:170:GLY:N	2:G:202:TYR:O	2.37	0.53
2:K:50:LEU:HD11	2:K:113:ILE:CG1	2.38	0.53
2:K:164:LEU:HD12	2:K:210:MET:HE1	1.89	0.53
1:E:63:GLU:C	1:E:64:VAL:HG13	2.34	0.53
1:E:232:SER:HB2	1:F:150:LEU:CD2	2.38	0.53
1:F:46:ASN:HD22	1:F:111:VAL:HG12	1.73	0.53
3:H:168:SER:O	3:H:203:ALA:HB1	2.09	0.53
1:J:220:SER:HA	1:J:231:GLU:HA	1.91	0.53
2:K:41:LEU:HD21	2:K:227:LEU:CD2	2.38	0.53
2:K:175:PRO:HD3	2:K:202:TYR:HB2	1.91	0.53
2:K:180:SER:OG	2:K:221:ILE:HD12	2.09	0.53
3:L:116:VAL:HG22	3:L:143:VAL:HG21	1.90	0.53
3:L:209:ILE:HG22	3:L:210:MET:N	2.23	0.53
1:E:162:ARG:NH1	1:E:164:GLU:OE1	2.42	0.53
1:E:235:PHE:HB2	1:F:153:MET:O	2.09	0.53
1:F:42:THR:OG1	1:F:45:GLU:OE1	2.27	0.53
1:F:220:SER:HA	1:F:231:GLU:HA	1.89	0.53
1:E:76:PHE:HB3	1:E:110:LEU:HD21	1.91	0.53
1:E:194:MET:C	1:E:201:PHE:HA	2.34	0.53
1:E:62:MET:HG2	1:E:64:VAL:HG22	1.91	0.53
1:E:178:TRP:CE2	1:E:205:THR:HG21	2.44	0.53
1:E:217:MET:C	1:E:234:ILE:HG22	2.34	0.53
1:E:235:PHE:O	1:F:153:MET:SD	2.67	0.53
1:E:237:PRO:HD3	1:F:155:GLY:HA3	1.91	0.53
2:G:111:LEU:HG	2:G:113:ILE:HD11	1.90	0.53
3:H:167:ARG:HA	3:H:205:ALA:HA	1.91	0.53
1:I:68:ARG:NH1	1:I:119:GLU:O	2.41	0.53
2:K:76:VAL:HG12	2:K:111:LEU:HD21	1.90	0.53
1:E:46:ASN:OD1	1:E:111:VAL:HG12	2.09	0.52
1:E:164:GLU:CB	1:E:206:ALA:HA	2.39	0.52
1:E:235:PHE:HB3	1:F:154:ARG:CD	2.38	0.52
1:I:121:GLY:N	1:I:140:LEU:O	2.41	0.52
2:K:150:LEU:HD21	2:K:231:LYS:HB3	1.91	0.52
1:F:149:PRO:HG3	1:F:230:LYS:C	2.34	0.52
1:F:153:MET:HB2	1:F:163:LEU:HA	1.90	0.52
1:F:214:VAL:O	1:F:236:ILE:HB	2.09	0.52
1:J:117:ALA:HB1	1:J:171:TYR:HB3	1.91	0.52
1:E:208:ILE:HB	1:E:210:ARG:CZ	2.40	0.52
1:I:123:TYR:CE1	1:I:140:LEU:HD13	2.44	0.52
1:E:64:VAL:HG21	1:E:128:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ARG:HG2	1:E:126:TYR:CE1	2.44	0.52
1:E:112:ILE:HD12	1:E:140:LEU:HD11	1.91	0.52
1:E:148:LYS:HB3	1:F:150:LEU:CD2	2.36	0.52
1:E:170:TRP:CD1	1:E:203:VAL:HB	2.45	0.52
1:E:189:LEU:N	1:E:206:ALA:O	2.34	0.52
1:J:148:LYS:O	1:J:167:SER:OG	2.26	0.52
2:K:42:ALA:N	2:K:142:LYS:O	2.43	0.52
3:L:59:SER:OG	3:L:61:GLU:OE1	2.26	0.52
3:L:135:GLU:OE1	3:L:135:GLU:N	2.42	0.52
3:L:176:GLN:NE2	3:L:225:SER:OG	2.42	0.52
1:E:50:ARG:HA	1:E:109:ALA:HA	1.90	0.52
1:E:148:LYS:HD3	1:E:230:LYS:HA	1.92	0.52
1:E:228:GLN:HG3	1:E:230:LYS:HG2	1.90	0.52
1:F:214:VAL:O	1:F:215:ARG:NH2	2.43	0.52
1:F:150:LEU:HB3	1:F:166:ILE:HB	1.90	0.52
1:F:221:ILE:O	1:F:229:LYS:HA	2.09	0.52
3:L:44:VAL:CG2	3:L:118:ALA:HB2	2.38	0.52
3:L:177:ILE:HA	3:L:221:THR:O	2.09	0.52
3:L:199:VAL:HG22	3:L:199:VAL:O	2.09	0.52
1:E:119:GLU:HB2	1:E:142:VAL:CG2	2.40	0.52
1:E:138:LEU:HD23	1:E:138:LEU:O	2.10	0.52
2:K:172:TYR:HA	2:K:173:PRO:C	2.35	0.52
3:L:170:GLY:N	3:L:202:TYR:O	2.42	0.52
1:E:228:GLN:O	1:E:230:LYS:N	2.41	0.52
1:F:154:ARG:HB2	1:F:162:ARG:HG3	1.92	0.52
1:F:157:GLU:OE2	1:F:208:ILE:HG23	2.10	0.52
2:G:178:GLN:HG2	2:G:221:ILE:HB	1.91	0.52
2:K:171:TRP:CB	2:K:175:PRO:HD3	2.40	0.52
1:E:180:ASP:OD1	1:E:216:ASN:O	2.26	0.52
1:F:129:GLU:HB3	2:G:129:GLN:HB3	1.92	0.52
1:F:219:CYS:O	1:F:232:SER:N	2.43	0.52
3:H:50:LEU:HD12	3:H:111:LEU:HD22	1.92	0.52
1:I:172:PRO:CG	1:I:225:LEU:HD12	2.39	0.52
1:J:162:ARG:HA	1:J:208:ILE:HA	1.90	0.52
1:E:47:THR:H	1:E:112:ILE:HB	1.75	0.52
1:E:216:ASN:HA	1:E:234:ILE:O	2.10	0.52
1:I:39:ILE:O	1:I:41:ALA:N	2.43	0.52
1:I:153:MET:SD	1:J:237:PRO:HD3	2.50	0.52
1:I:233:VAL:HG12	1:I:234:ILE:N	2.24	0.52
1:J:66:TRP:HE1	1:J:125:CYS:HA	1.75	0.52
1:E:232:SER:OG	1:F:150:LEU:HD22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:PRO:HB2	1:F:129:GLU:OE1	2.10	0.51
1:E:117:ALA:O	1:E:171:TYR:CZ	2.63	0.51
1:E:153:MET:O	1:F:235:PHE:CB	2.58	0.51
1:E:45:GLU:OE2	1:E:47:THR:OG1	2.29	0.51
1:E:125:CYS:H	1:E:136:ALA:HB3	1.74	0.51
1:E:178:TRP:NE1	1:E:207:VAL:HG11	2.25	0.51
1:E:178:TRP:CZ2	1:E:205:THR:HG21	2.45	0.51
1:I:112:ILE:CG2	1:I:115:ILE:HD11	2.40	0.51
1:J:68:ARG:O	1:J:124:ARG:CG	2.59	0.51
2:K:209:ILE:HG22	2:K:210:MET:N	2.24	0.51
3:L:46:GLU:O	3:L:116:VAL:N	2.33	0.51
1:F:162:ARG:HA	1:F:208:ILE:HA	1.93	0.51
1:J:45:GLU:O	1:J:114:ASN:N	2.43	0.51
2:G:162:ILE:HD12	2:G:237:ILE:HB	1.92	0.51
3:L:172:TYR:HE1	3:L:226:LEU:HD22	1.76	0.51
1:E:188:ALA:CA	1:E:207:VAL:HG12	2.39	0.51
2:K:192:ALA:N	2:K:205:ALA:O	2.44	0.51
3:L:162:ILE:HG22	3:L:163:HIS:N	2.25	0.51
2:G:68:VAL:HG12	2:G:75:VAL:HB	1.92	0.51
2:G:172:TYR:CZ	2:G:200:GLY:O	2.63	0.51
1:I:100:SER:O	1:I:103:ILE:HG22	2.11	0.51
1:J:49:LEU:HD11	1:J:123:TYR:HD2	1.76	0.51
3:L:37:SER:HA	3:L:138:LEU:HD12	1.93	0.51
3:L:124:TYR:N	3:L:139:VAL:O	2.31	0.51
3:L:204:VAL:HG21	3:L:222:ILE:HD13	1.92	0.51
1:E:95:ARG:O	1:E:113:HIS:ND1	2.44	0.51
1:F:65:ARG:NH2	1:F:72:SER:HA	2.26	0.51
1:F:214:VAL:HG13	1:F:236:ILE:HG13	1.92	0.51
1:F:216:ASN:HA	1:F:235:PHE:HA	1.92	0.51
1:J:66:TRP:O	1:J:74:ALA:HB1	2.10	0.51
1:J:163:LEU:HD12	1:J:234:ILE:HG21	1.92	0.51
2:K:68:VAL:HG12	2:K:75:VAL:HG22	1.92	0.51
1:E:149:PRO:HG3	1:E:221:ILE:N	2.26	0.51
1:E:165:CYS:SG	1:E:205:THR:HG22	2.50	0.51
1:F:217:MET:N	1:F:234:ILE:O	2.44	0.51
2:G:75:VAL:HG13	2:G:75:VAL:O	2.10	0.51
3:H:177:ILE:HG23	3:H:189:THR:CG2	2.41	0.51
1:I:223:ASN:OD1	1:I:225:LEU:N	2.43	0.51
2:K:123:LYS:HG3	2:K:140:GLU:HG2	1.93	0.51
2:K:184:GLY:C	2:K:221:ILE:HD11	2.36	0.51
1:E:123:TYR:HB2	1:E:138:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:LEU:HD12	1:F:226:LEU:HG	1.93	0.51
3:L:42:ALA:O	3:L:143:VAL:HA	2.11	0.51
3:L:235:ILE:HG22	3:L:236:SER:N	2.26	0.51
1:E:42:THR:HG22	1:E:43:VAL:N	2.21	0.50
1:J:110:LEU:HG	1:J:112:ILE:HD11	1.92	0.50
2:K:78:VAL:HG21	2:K:88:ARG:HE	1.76	0.50
2:K:179:TRP:N	2:K:191:GLU:OE2	2.44	0.50
3:L:152:VAL:HG12	3:L:153:ASP:N	2.27	0.50
1:E:39:ILE:O	1:E:140:LEU:HG	2.11	0.50
1:E:122:THR:HA	1:E:139:HIS:HA	1.93	0.50
2:G:64:GLU:OE1	2:G:65:LEU:N	2.38	0.50
2:K:150:LEU:HD21	2:K:231:LYS:CB	2.41	0.50
2:K:162:ILE:HB	2:K:237:ILE:HG22	1.93	0.50
1:E:63:GLU:O	1:E:64:VAL:HG13	2.11	0.50
1:E:162:ARG:HA	1:E:208:ILE:HA	1.93	0.50
1:E:181:PRO:N	1:E:216:ASN:HB2	2.27	0.50
3:H:166:CYS:O	3:H:206:ALA:N	2.44	0.50
2:K:47:ASP:OD1	2:K:115:ASN:N	2.44	0.50
1:E:162:ARG:HA	1:E:208:ILE:HG12	1.92	0.50
1:F:163:LEU:HB3	1:F:178:TRP:CZ2	2.47	0.50
3:H:60:ALA:CB	3:H:63:MET:HE2	2.42	0.50
3:H:192:ALA:HB1	3:H:193:PRO:CD	2.41	0.50
1:I:147:SER:OG	1:J:149:PRO:O	2.30	0.50
1:F:68:ARG:HD2	1:F:68:ARG:O	2.11	0.50
1:F:217:MET:HB3	1:F:234:ILE:CG2	2.42	0.50
2:G:68:VAL:O	2:G:69:SER:C	2.54	0.50
2:G:100:LEU:HD11	2:G:112:ARG:HB2	1.93	0.50
2:G:118:ALA:HB3	2:G:199:VAL:HG22	1.93	0.50
2:K:76:VAL:HG12	2:K:111:LEU:CD2	2.42	0.50
2:K:113:ILE:HG21	2:K:116:VAL:HG22	1.93	0.50
3:L:144:ALA:HA	3:L:172:TYR:CE1	2.47	0.50
1:E:234:ILE:HA	1:F:152:SER:CA	2.42	0.50
1:F:156:HIS:HA	1:F:160:GLY:C	2.37	0.50
2:G:221:ILE:HD11	2:G:232:THR:HG23	1.93	0.50
3:H:145:ALA:C	3:H:146:LEU:HD22	2.36	0.50
1:I:222:ASN:OD1	1:I:223:ASN:N	2.45	0.50
2:K:146:LEU:HD22	2:K:229:LEU:HB3	1.93	0.50
3:L:33:VAL:O	3:L:136:LYS:HB2	2.12	0.50
1:E:63:GLU:OE1	3:L:134:TYR:HB3	2.12	0.50
1:E:116:THR:HA	1:E:198:ASP:HB2	1.93	0.50
1:E:117:ALA:HB1	1:E:171:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:PRO:HG2	1:E:240:PHE:CZ	2.47	0.50
1:I:41:ALA:HB3	1:I:142:VAL:HG22	1.94	0.50
1:I:42:THR:HG22	1:I:43:VAL:N	2.27	0.50
1:I:153:MET:SD	1:J:237:PRO:CD	3.00	0.50
3:L:123:LYS:HA	3:L:140:GLU:HA	1.94	0.50
1:E:166:ILE:HD12	1:F:233:VAL:HB	1.93	0.50
1:E:178:TRP:HA	1:E:219:CYS:HA	1.94	0.50
1:F:176:THR:HA	1:F:221:ILE:HA	1.94	0.50
1:E:64:VAL:HG23	1:E:127:PHE:HA	1.94	0.50
1:E:109:ALA:O	1:E:110:LEU:HD12	2.11	0.50
1:E:120:ASN:CG	1:E:141:VAL:HG23	2.37	0.50
1:E:142:VAL:HB	1:E:171:TYR:CE1	2.47	0.50
1:E:219:CYS:O	1:E:232:SER:N	2.41	0.50
2:G:178:GLN:HB2	2:G:187:ILE:O	2.11	0.50
1:I:153:MET:CB	1:I:163:LEU:HA	2.42	0.50
1:E:170:TRP:CZ3	1:E:223:ASN:HB2	2.47	0.49
1:J:122:THR:HG23	1:J:138:LEU:O	2.12	0.49
1:J:149:PRO:HG2	1:J:230:LYS:O	2.12	0.49
1:J:170:TRP:CD1	1:J:203:VAL:HG22	2.47	0.49
3:L:54:LEU:HB2	3:L:57:THR:HA	1.93	0.49
1:E:41:ALA:HB3	1:E:142:VAL:CG2	2.34	0.49
2:G:168:SER:N	2:G:204:VAL:O	2.45	0.49
2:K:117:THR:N	2:K:120:ASP:OD2	2.40	0.49
3:L:67:TRP:CH2	3:L:139:VAL:HG21	2.47	0.49
1:E:39:ILE:HG22	1:E:47:THR:CG2	2.41	0.49
1:E:49:LEU:HD13	1:E:123:TYR:HD2	1.77	0.49
1:E:153:MET:HA	1:E:163:LEU:HA	1.93	0.49
1:F:150:LEU:N	1:F:166:ILE:O	2.45	0.49
1:F:156:HIS:HA	1:F:160:GLY:O	2.12	0.49
1:F:214:VAL:HG22	1:F:215:ARG:H	1.77	0.49
1:I:65:ARG:NH2	1:I:72:SER:OG	2.45	0.49
1:E:40:LEU:HD11	1:E:143:ALA:CB	2.39	0.49
1:I:188:ALA:HA	1:I:207:VAL:HG12	1.92	0.49
1:J:149:PRO:HA	1:J:167:SER:OG	2.13	0.49
3:L:36:PRO:HD2	3:L:139:VAL:HG22	1.93	0.49
1:E:66:TRP:HB2	1:E:76:PHE:O	2.13	0.49
1:J:151:ILE:HA	1:J:164:GLU:O	2.12	0.49
1:J:196:ASP:OD1	1:J:200:LEU:N	2.39	0.49
3:L:179:TRP:NE1	3:L:207:SER:O	2.44	0.49
1:E:35:PRO:HB2	1:E:39:ILE:HD11	1.93	0.49
2:G:47:ASP:OD1	2:G:115:ASN:N	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:PRO:CD	1:I:225:LEU:HD12	2.42	0.49
1:J:92:TYR:CD1	1:J:112:ILE:HG21	2.47	0.49
2:K:69:SER:HA	2:K:124:TYR:CE2	2.48	0.49
1:F:154:ARG:N	1:F:162:ARG:O	2.38	0.49
1:E:153:MET:N	1:E:164:GLU:OE2	2.46	0.49
1:E:170:TRP:HB2	1:E:202:MET:HA	1.95	0.49
1:E:180:ASP:CG	1:E:181:PRO:HD2	2.38	0.49
1:F:128:GLN:O	2:G:129:GLN:HB3	2.13	0.49
1:F:150:LEU:HD12	1:F:166:ILE:HG22	1.95	0.49
2:G:64:GLU:CD	2:G:65:LEU:H	2.18	0.49
2:G:235:ILE:HA	3:H:152:VAL:HG21	1.94	0.49
1:E:61:ASP:OD1	1:E:61:ASP:N	2.46	0.49
1:E:187:PRO:O	1:E:210:ARG:NH2	2.46	0.49
1:I:95:ARG:NH2	1:I:114:ASN:O	2.37	0.49
1:J:138:LEU:HD12	1:J:139:HIS:N	2.28	0.49
2:K:124:TYR:HB2	2:K:139:VAL:HB	1.94	0.49
3:L:39:PRO:HB2	3:L:142:LYS:HB2	1.93	0.49
3:L:63:MET:HG3	3:L:130:ASP:HB3	1.94	0.49
3:L:97:THR:HG22	3:L:113:ILE:HG23	1.95	0.49
1:E:149:PRO:HB2	1:E:232:SER:HB3	1.95	0.49
1:F:73:PRO:HA	1:F:87:GLU:HB3	1.95	0.49
3:H:48:ALA:CB	3:H:141:LEU:HD22	2.42	0.49
1:J:53:LEU:HD12	1:J:53:LEU:O	2.13	0.49
1:J:60:GLU:O	1:J:61:ASP:OD1	2.31	0.49
1:J:149:PRO:HB2	1:J:232:SER:CB	2.42	0.49
2:K:42:ALA:O	2:K:144:ALA:N	2.42	0.49
2:K:223:ARG:HA	2:K:230:GLU:HA	1.94	0.49
3:L:195:VAL:O	3:L:203:ALA:HB3	2.13	0.49
1:E:126:TYR:HA	1:E:134:ASP:O	2.12	0.48
2:G:194:VAL:HA	2:G:203:GLU:H	1.77	0.48
1:I:162:ARG:NE	1:I:206:ALA:HB1	2.28	0.48
1:J:179:ARG:O	1:J:218:SER:N	2.45	0.48
3:L:177:ILE:HB	3:L:204:VAL:HB	1.95	0.48
1:E:32:VAL:CG1	1:E:136:ALA:HB2	2.37	0.48
3:H:103:GLY:O	3:H:107:GLY:N	2.46	0.48
2:K:144:ALA:HB1	2:K:224:ASN:HD21	1.77	0.48
3:L:191:GLU:OE1	3:L:194:VAL:HG11	2.13	0.48
1:F:32:VAL:HG21	1:F:127:PHE:CE1	2.48	0.48
1:F:157:GLU:OE1	1:F:161:ILE:N	2.46	0.48
2:G:63:MET:CG	2:G:65:LEU:HB2	2.42	0.48
3:L:172:TYR:CE1	3:L:226:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:N	1:E:140:LEU:HA	2.28	0.48
1:E:42:THR:OG1	1:E:45:GLU:OE1	2.19	0.48
1:E:176:THR:HA	1:E:221:ILE:HA	1.95	0.48
1:E:233:VAL:O	1:F:152:SER:HB2	2.13	0.48
1:F:67:PHE:O	1:F:126:TYR:HB3	2.13	0.48
1:I:149:PRO:HA	1:I:167:SER:OG	2.14	0.48
1:J:89:MET:HE1	1:J:116:THR:HG22	1.91	0.48
1:J:158:ASP:OD1	1:J:158:ASP:N	2.46	0.48
1:J:163:LEU:HB3	1:J:178:TRP:CH2	2.49	0.48
3:L:67:TRP:NE1	3:L:109:ALA:O	2.44	0.48
1:E:64:VAL:HG11	1:E:128:GLN:HG2	1.94	0.48
1:E:67:PHE:CA	1:E:75:VAL:HG22	2.43	0.48
1:E:216:ASN:OD1	1:E:235:PHE:N	2.46	0.48
1:F:171:TYR:O	1:F:226:LEU:HD11	2.14	0.48
2:K:133:PHE:O	2:K:135:GLU:HA	2.13	0.48
2:K:168:SER:HB3	2:K:222:ILE:HG21	1.95	0.48
3:L:116:VAL:HG13	3:L:116:VAL:O	2.13	0.48
3:L:192:ALA:HB1	3:L:193:PRO:CD	2.44	0.48
1:E:194:MET:O	1:E:202:MET:N	2.47	0.48
1:F:115:ILE:HG22	1:F:142:VAL:HG11	1.95	0.48
2:G:146:LEU:HD12	2:G:171:TRP:HZ3	1.78	0.48
3:H:42:ALA:O	3:H:143:VAL:HG22	2.14	0.48
1:J:89:MET:O	1:J:93:ARG:NE	2.37	0.48
3:L:31:PHE:CG	3:L:130:ASP:OD1	2.67	0.48
1:E:67:PHE:HB2	1:E:70:GLN:O	2.13	0.48
1:E:154:ARG:HA	1:F:235:PHE:CD2	2.49	0.48
1:I:152:SER:HA	1:J:234:ILE:HG13	1.96	0.48
1:I:166:ILE:HG22	1:I:167:SER:N	2.27	0.48
1:J:125:CYS:O	1:J:136:ALA:HB3	2.14	0.48
1:J:128:GLN:O	2:K:134:TYR:CD1	2.67	0.48
1:E:157:GLU:OE2	1:E:162:ARG:HB2	2.14	0.48
1:E:166:ILE:HA	1:E:204:THR:HG23	1.95	0.48
1:F:91:GLU:HB3	1:F:116:THR:HB	1.95	0.48
1:F:144:GLY:N	1:F:171:TYR:O	2.45	0.48
1:I:220:SER:OG	1:I:231:GLU:HG3	2.13	0.48
1:J:218:SER:HA	1:J:233:VAL:HA	1.96	0.48
1:E:143:ALA:HA	1:E:171:TYR:O	2.13	0.48
1:F:189:LEU:HD21	1:F:208:ILE:HG13	1.94	0.48
2:G:177:ILE:CG2	2:G:190:VAL:O	2.62	0.48
1:J:193:SER:OG	1:J:201:PHE:HB3	2.14	0.48
2:K:123:LYS:HD2	2:K:141:LEU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:LEU:HD13	3:L:139:VAL:CG1	2.43	0.48
1:F:95:ARG:HD3	1:F:114:ASN:CB	2.44	0.48
1:I:105:ARG:NH2	1:I:107:SER:O	2.46	0.48
1:J:49:LEU:HD11	1:J:123:TYR:CD2	2.48	0.48
1:J:66:TRP:NE1	1:J:125:CYS:HA	2.29	0.48
1:J:123:TYR:HB2	1:J:138:LEU:HD11	1.96	0.48
1:E:49:LEU:CD1	1:E:123:TYR:HD2	2.27	0.47
1:J:212:LYS:HB3	1:J:238:GLU:HB3	1.95	0.47
3:L:36:PRO:HG2	3:L:139:VAL:HG13	1.96	0.47
3:L:54:LEU:HD23	3:L:130:ASP:OD2	2.13	0.47
1:E:62:MET:HE1	1:E:127:PHE:CD1	2.50	0.47
1:E:153:MET:C	1:E:164:GLU:OE1	2.57	0.47
1:E:214:VAL:O	1:E:236:ILE:HB	2.14	0.47
1:F:74:ALA:N	1:F:87:GLU:O	2.45	0.47
1:F:164:GLU:HB3	1:F:190:LYS:HG3	1.95	0.47
1:I:164:GLU:HG2	1:I:206:ALA:HB2	1.96	0.47
2:K:134:TYR:O	2:K:134:TYR:CG	2.67	0.47
2:K:146:LEU:O	2:K:170:GLY:O	2.32	0.47
1:E:123:TYR:CZ	1:E:140:LEU:HB3	2.48	0.47
1:E:152:SER:CB	1:F:234:ILE:HA	2.44	0.47
1:F:91:GLU:CD	1:F:116:THR:HG22	2.39	0.47
1:F:117:ALA:HB3	1:F:199:GLY:O	2.14	0.47
1:F:219:CYS:HB3	1:F:232:SER:OG	2.14	0.47
2:G:152:VAL:HG22	2:G:153:GLU:H	1.80	0.47
1:I:170:TRP:HB3	1:I:174:PRO:CG	2.44	0.47
1:J:220:SER:HA	1:J:230:LYS:O	2.13	0.47
2:K:157:TYR:OH	2:K:159:ASP:O	2.25	0.47
3:L:68:VAL:HG13	3:L:74:GLN:C	2.39	0.47
1:E:70:GLN:CD	1:E:89:MET:SD	2.97	0.47
1:E:77:VAL:HG12	1:E:78:TYR:N	2.30	0.47
1:E:179:ARG:HB2	1:E:218:SER:HB3	1.95	0.47
1:F:154:ARG:HG2	1:F:190:LYS:HD3	1.96	0.47
3:H:169:THR:OG1	3:H:170:GLY:N	2.48	0.47
1:J:59:ALA:HB3	1:J:103:ILE:CD1	2.44	0.47
1:J:60:GLU:O	1:J:78:TYR:CZ	2.67	0.47
3:L:196:ALA:HA	3:L:202:TYR:HA	1.96	0.47
1:E:120:ASN:N	1:E:142:VAL:HG23	2.30	0.47
1:F:117:ALA:HB1	1:F:171:TYR:HB3	1.97	0.47
1:F:217:MET:HB3	1:F:234:ILE:O	2.15	0.47
1:F:219:CYS:N	1:F:232:SER:O	2.47	0.47
1:I:75:VAL:HG11	1:I:110:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:71:SER:OG	2:K:123:LYS:HD3	2.15	0.47
1:E:223:ASN:O	1:E:227:GLY:N	2.45	0.47
1:F:170:TRP:CZ3	1:F:226:LEU:HD13	2.50	0.47
2:G:33:VAL:HG22	2:G:52:CYS:HA	1.95	0.47
2:G:68:VAL:HG12	2:G:75:VAL:HA	1.97	0.47
2:G:152:VAL:HG22	2:G:153:GLU:N	2.29	0.47
2:K:146:LEU:HD13	2:K:229:LEU:C	2.40	0.47
3:L:169:THR:HA	3:L:203:ALA:CB	2.45	0.47
3:L:234:SER:O	3:L:235:ILE:HD13	2.14	0.47
1:E:171:TYR:HB2	1:E:200:LEU:HG	1.96	0.47
2:G:37:SER:CB	2:G:139:VAL:HG22	2.45	0.47
2:G:60:ALA:N	2:G:63:MET:HE1	2.29	0.47
2:G:85:VAL:O	2:G:85:VAL:HG13	2.15	0.47
2:G:146:LEU:HD11	2:G:229:LEU:HB2	1.95	0.47
2:G:208:VAL:HG11	2:G:218:VAL:CG2	2.45	0.47
3:H:153:ASP:OD1	3:H:154:VAL:N	2.45	0.47
1:I:147:SER:OG	1:J:148:LYS:HB3	2.14	0.47
1:J:40:LEU:HD12	1:J:143:ALA:CA	2.44	0.47
2:K:54:LEU:HD12	2:K:107:GLY:O	2.14	0.47
2:K:84:GLU:HG3	2:K:99:ILE:HD12	1.97	0.47
2:K:96:ARG:O	2:K:114:HIS:N	2.47	0.47
2:K:146:LEU:HD13	2:K:229:LEU:HB3	1.96	0.47
3:L:67:TRP:O	3:L:77:ASN:O	2.33	0.47
3:L:67:TRP:HB3	3:L:76:VAL:HG13	1.96	0.47
1:E:53:LEU:O	1:E:107:SER:OG	2.32	0.47
1:E:148:LYS:HB2	1:F:149:PRO:O	2.15	0.47
1:E:162:ARG:HG2	1:E:189:LEU:HD11	1.96	0.47
1:E:222:ASN:HA	1:E:229:LYS:HA	1.97	0.47
1:E:234:ILE:HD11	1:F:153:MET:HE3	1.95	0.47
2:G:50:LEU:HD22	2:G:124:TYR:CD2	2.50	0.47
1:J:97:THR:OG1	1:J:111:VAL:HB	2.14	0.47
1:E:35:PRO:HD2	1:E:50:ARG:O	2.15	0.47
1:E:115:ILE:HG22	1:E:117:ALA:N	2.30	0.47
1:E:180:ASP:OD1	1:E:181:PRO:HD3	2.15	0.47
1:F:41:ALA:C	1:F:142:VAL:HG13	2.40	0.47
1:F:95:ARG:HB3	1:F:113:HIS:HB2	1.96	0.47
1:F:215:ARG:HB3	1:F:235:PHE:CZ	2.50	0.47
1:I:178:TRP:CZ2	1:I:207:VAL:HG13	2.50	0.47
1:I:214:VAL:O	1:I:215:ARG:NH2	2.48	0.47
1:J:149:PRO:HG3	1:J:221:ILE:HG22	1.97	0.47
1:J:214:VAL:HG23	1:J:236:ILE:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:44:VAL:CG2	2:K:118:ALA:HB2	2.45	0.47
1:E:218:SER:CB	1:E:233:VAL:HA	2.45	0.47
1:F:152:SER:HB3	1:F:164:GLU:HG3	1.95	0.47
2:G:68:VAL:HG12	2:G:75:VAL:CB	2.45	0.47
1:I:123:TYR:HB2	1:I:138:LEU:HD22	1.97	0.47
1:J:174:PRO:HA	1:J:223:ASN:HA	1.97	0.47
1:J:192:VAL:O	1:J:192:VAL:HG13	2.15	0.47
2:K:118:ALA:O	2:K:172:TYR:CD1	2.68	0.47
2:K:168:SER:O	2:K:203:GLU:HA	2.15	0.47
3:L:144:ALA:HB3	3:L:227:LEU:HD11	1.97	0.47
1:F:166:ILE:HD13	1:F:204:THR:CB	2.44	0.46
1:E:149:PRO:HD3	1:E:230:LYS:O	2.15	0.46
1:F:70:GLN:HB2	1:F:73:PRO:HG2	1.96	0.46
1:F:164:GLU:HA	1:F:205:THR:O	2.13	0.46
3:H:50:LEU:HD12	3:H:111:LEU:HB3	1.96	0.46
1:J:116:THR:CG2	1:J:119:GLU:HG3	2.45	0.46
1:J:215:ARG:O	1:J:235:PHE:HA	2.14	0.46
2:K:170:GLY:HA2	2:K:201:LEU:HB3	1.96	0.46
3:L:89:GLN:NE2	3:L:97:THR:O	2.48	0.46
1:E:146:GLY:HA2	1:E:168:ARG:O	2.15	0.46
2:G:63:MET:HA	2:G:64:GLU:HB3	1.96	0.46
2:G:96:ARG:O	2:G:114:HIS:N	2.45	0.46
2:G:179:TRP:CZ2	2:G:206:ALA:HB3	2.50	0.46
1:I:235:PHE:HB2	1:J:153:MET:O	2.15	0.46
1:J:42:THR:O	1:J:115:ILE:N	2.42	0.46
1:J:154:ARG:HB3	1:J:162:ARG:HB3	1.96	0.46
3:L:177:ILE:HD11	3:L:220:CYS:SG	2.56	0.46
1:E:53:LEU:HD22	1:E:106:GLY:CA	2.45	0.46
1:F:186:ALA:HB1	1:F:207:VAL:HB	1.98	0.46
1:I:217:MET:H	1:I:234:ILE:HG23	1.79	0.46
2:K:89:GLN:HB2	2:K:94:ARG:HA	1.96	0.46
3:L:223:ARG:HB2	3:L:230:GLU:HG2	1.98	0.46
1:E:38:PRO:HB2	1:E:141:VAL:HG12	1.98	0.46
1:E:159:GLY:O	1:E:240:PHE:CE2	2.69	0.46
1:F:123:TYR:CD2	1:F:140:LEU:HD23	2.50	0.46
1:F:178:TRP:CD1	1:F:186:ALA:HB3	2.50	0.46
1:E:70:GLN:O	1:E:74:ALA:CB	2.62	0.46
1:E:149:PRO:HB2	1:E:232:SER:CB	2.45	0.46
1:E:237:PRO:HG3	1:F:156:HIS:N	2.31	0.46
1:J:118:GLN:HA	1:J:171:TYR:CZ	2.50	0.46
3:L:109:ALA:HB2	3:L:128:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:171:TRP:HB3	3:L:175:PRO:CD	2.46	0.46
3:L:171:TRP:HB3	3:L:175:PRO:HG3	1.98	0.46
3:L:178:GLN:O	3:L:221:THR:N	2.47	0.46
1:F:42:THR:N	1:F:45:GLU:HB2	2.30	0.46
2:G:191:GLU:OE1	2:G:204:VAL:HG21	2.16	0.46
3:H:124:TYR:HE1	3:H:141:LEU:HD23	1.81	0.46
1:I:214:VAL:CG1	1:I:217:MET:HE2	2.40	0.46
1:J:110:LEU:CG	1:J:112:ILE:HD11	2.46	0.46
1:E:173:LYS:N	1:E:174:PRO:HD3	2.31	0.46
1:E:244:VAL:HG12	1:F:243:SER:CB	2.46	0.46
1:F:151:ILE:HG21	1:F:234:ILE:CG2	2.46	0.46
3:H:60:ALA:HB2	3:H:63:MET:HE2	1.97	0.46
3:H:177:ILE:HG21	3:H:204:VAL:HB	1.98	0.46
1:I:44:GLY:HA2	1:I:114:ASN:HA	1.98	0.46
1:J:117:ALA:CB	1:J:171:TYR:HB3	2.46	0.46
1:J:189:LEU:HG	1:J:206:ALA:O	2.15	0.46
3:L:145:ALA:HB3	3:L:172:TYR:CB	2.46	0.46
1:E:75:VAL:CG1	1:E:89:MET:HE2	2.41	0.46
1:E:176:THR:HG23	1:E:219:CYS:SG	2.56	0.46
1:I:149:PRO:HB2	1:I:232:SER:OG	2.16	0.46
1:J:151:ILE:HD13	1:J:234:ILE:CG2	2.42	0.46
2:K:67:TRP:NE1	2:K:111:LEU:HB3	2.31	0.46
2:K:96:ARG:O	2:K:114:HIS:ND1	2.47	0.46
2:K:208:VAL:HG11	2:K:218:VAL:HG11	1.97	0.46
1:E:49:LEU:HB3	1:E:110:LEU:O	2.16	0.46
1:E:65:ARG:HD3	1:E:74:ALA:HB2	1.98	0.46
1:E:95:ARG:O	1:E:113:HIS:N	2.49	0.46
1:E:150:LEU:HD21	1:F:149:PRO:HG2	1.97	0.46
1:E:174:PRO:HG3	1:E:223:ASN:ND2	2.31	0.46
1:E:193:SER:OG	1:E:201:PHE:O	2.34	0.46
1:E:244:VAL:HG12	1:F:243:SER:HB3	1.97	0.46
1:F:182:TYR:CD1	1:F:214:VAL:HG23	2.51	0.46
2:G:37:SER:CA	2:G:139:VAL:HG22	2.46	0.46
3:H:49:ASP:OD1	3:H:49:ASP:N	2.49	0.46
1:J:125:CYS:SG	1:J:127:PHE:CG	3.09	0.46
2:K:146:LEU:HD13	2:K:229:LEU:CB	2.46	0.46
2:K:179:TRP:O	2:K:180:SER:OG	2.29	0.46
3:L:167:ARG:HA	3:L:205:ALA:HA	1.98	0.46
3:L:178:GLN:HA	3:L:189:THR:CB	2.45	0.46
1:E:40:LEU:O	1:E:45:GLU:OE1	2.34	0.45
1:E:46:ASN:HA	1:E:113:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LEU:HG	1:E:49:LEU:O	2.16	0.45
1:E:57:LYS:NZ	1:E:62:MET:SD	2.87	0.45
1:E:57:LYS:N	1:E:105:ARG:O	2.49	0.45
1:E:153:MET:O	1:E:164:GLU:OE2	2.34	0.45
1:E:179:ARG:CZ	1:E:231:GLU:HB2	2.47	0.45
2:G:69:SER:OG	2:G:76:VAL:HG13	2.16	0.45
1:J:150:LEU:HD11	1:J:166:ILE:HB	1.99	0.45
2:K:43:MET:SD	2:K:227:LEU:HD11	2.56	0.45
1:E:48:THR:O	1:E:140:LEU:HD12	2.16	0.45
1:F:241:MET:SD	1:F:242:PRO:O	2.74	0.45
2:G:50:LEU:N	2:G:50:LEU:HD12	2.31	0.45
1:I:145:LEU:HA	1:I:170:TRP:CE3	2.51	0.45
1:I:148:LYS:HB3	1:J:150:LEU:HD23	1.98	0.45
1:I:172:PRO:HA	1:I:201:PHE:HB2	1.98	0.45
1:I:190:LYS:O	1:I:206:ALA:N	2.50	0.45
2:K:43:MET:HA	2:K:144:ALA:O	2.17	0.45
2:K:72:LEU:HD11	2:K:121:SER:N	2.32	0.45
3:L:50:LEU:HD12	3:L:111:LEU:HD23	1.98	0.45
1:E:148:LYS:CB	1:F:150:LEU:CD2	2.94	0.45
1:E:151:ILE:HA	1:E:165:CYS:CA	2.46	0.45
1:E:218:SER:C	1:E:232:SER:O	2.59	0.45
1:F:35:PRO:HG3	1:F:49:LEU:HD23	1.98	0.45
1:F:158:ASP:OD1	1:F:210:ARG:NE	2.49	0.45
3:H:150:LEU:HD12	3:H:166:CYS:HB2	1.97	0.45
1:I:106:GLY:O	1:I:108:VAL:HG13	2.17	0.45
1:J:167:SER:HB2	1:J:170:TRP:HE1	1.82	0.45
3:L:44:VAL:HG13	3:L:118:ALA:H	1.81	0.45
1:E:92:TYR:HE2	1:E:123:TYR:CE2	2.35	0.45
1:E:119:GLU:HB2	1:E:142:VAL:HG21	1.99	0.45
1:F:178:TRP:NE1	1:F:205:THR:O	2.48	0.45
2:G:175:PRO:HD3	2:G:202:TYR:HB2	1.98	0.45
3:H:192:ALA:HB3	3:H:205:ALA:HB1	1.97	0.45
1:I:49:LEU:HA	1:I:138:LEU:HD13	1.98	0.45
1:I:153:MET:HB3	1:I:163:LEU:HA	1.97	0.45
1:E:33:VAL:HG23	1:E:52:HIS:HB2	1.99	0.45
1:E:150:LEU:HD13	1:F:232:SER:HA	1.99	0.45
1:F:188:ALA:HA	1:F:206:ALA:H	1.80	0.45
1:J:53:LEU:HB3	1:J:127:PHE:CZ	2.52	0.45
1:J:65:ARG:NH2	1:J:70:GLN:O	2.46	0.45
1:J:65:ARG:HA	1:J:77:VAL:HA	1.97	0.45
2:K:175:PRO:CD	2:K:202:TYR:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:VAL:HG12	3:L:79:TYR:N	2.31	0.45
3:L:145:ALA:HB3	3:L:172:TYR:HB3	1.97	0.45
1:E:234:ILE:HD11	1:F:153:MET:CE	2.47	0.45
1:F:209:ILE:HG22	1:F:211:ASP:H	1.81	0.45
3:H:145:ALA:N	3:H:172:TYR:O	2.44	0.45
1:I:39:ILE:HD12	1:I:138:LEU:HD21	1.98	0.45
1:J:123:TYR:CE2	1:J:140:LEU:HD23	2.52	0.45
3:L:70:SER:H	3:L:124:TYR:HA	1.82	0.45
3:L:166:CYS:SG	3:L:206:ALA:HB3	2.57	0.45
1:E:57:LYS:HD2	1:E:129:GLU:HA	1.98	0.45
1:E:63:GLU:O	1:E:64:VAL:CG1	2.65	0.45
1:E:149:PRO:N	1:F:150:LEU:CD2	2.80	0.45
1:E:157:GLU:N	1:E:160:GLY:O	2.35	0.45
1:E:222:ASN:HA	1:E:228:GLN:O	2.16	0.45
1:E:235:PHE:HB2	1:F:164:GLU:OE2	2.16	0.45
1:F:41:ALA:CB	1:F:115:ILE:HD12	2.46	0.45
3:H:50:LEU:HA	3:H:139:VAL:HG11	1.98	0.45
1:I:105:ARG:HH12	1:I:107:SER:C	2.25	0.45
1:I:174:PRO:HB3	1:I:223:ASN:HA	1.99	0.45
2:K:113:ILE:HG22	2:K:114:HIS:N	2.31	0.45
2:K:165:GLU:HG3	2:K:206:ALA:O	2.17	0.45
2:K:172:TYR:CG	2:K:173:PRO:HA	2.52	0.45
3:L:67:TRP:CE2	3:L:111:LEU:HB2	2.51	0.45
3:L:112:ARG:CZ	3:L:112:ARG:HB2	2.47	0.45
3:L:161:GLY:O	3:L:162:ILE:HD13	2.16	0.45
1:E:66:TRP:HB2	1:E:75:VAL:O	2.16	0.45
1:E:124:ARG:HD2	1:E:135:GLU:OE2	2.17	0.45
1:E:239:SER:C	1:E:240:PHE:CD1	2.95	0.45
1:F:209:ILE:HG22	1:F:211:ASP:N	2.32	0.45
3:H:178:GLN:HB2	3:H:221:THR:OG1	2.16	0.45
2:K:42:ALA:HB1	2:K:46:GLU:HB2	1.98	0.45
1:E:98:PHE:HD1	1:E:110:LEU:HD11	1.80	0.45
1:E:169:GLY:O	1:E:200:LEU:HD21	2.16	0.45
1:E:240:PHE:CD2	1:F:156:HIS:CD2	3.04	0.45
1:F:175:LEU:HB2	1:F:222:ASN:O	2.17	0.45
1:F:190:LYS:HG3	1:F:190:LYS:O	2.17	0.45
2:G:52:CYS:H	2:G:110:ALA:HA	1.81	0.45
2:G:147:GLY:O	2:G:148:SER:OG	2.26	0.45
1:I:151:ILE:HB	1:J:151:ILE:O	2.16	0.45
1:J:31:ILE:O	1:J:52:HIS:NE2	2.50	0.45
1:J:126:TYR:HB3	2:K:134:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:117:THR:O	2:K:143:VAL:HG11	2.17	0.45
2:K:190:VAL:HG13	2:K:190:VAL:O	2.16	0.45
1:E:151:ILE:HG23	1:E:178:TRP:CH2	2.52	0.45
1:E:162:ARG:O	1:E:162:ARG:CD	2.65	0.45
1:F:65:ARG:HB2	2:G:134:TYR:CE1	2.52	0.45
2:G:104:ILE:O	2:G:104:ILE:HG23	2.16	0.45
1:I:46:ASN:OD1	1:I:113:HIS:ND1	2.50	0.45
1:J:103:ILE:HD12	1:J:106:GLY:HA2	1.99	0.45
2:K:50:LEU:HD12	2:K:67:TRP:HE1	1.81	0.45
2:K:150:LEU:HA	2:K:167:ARG:O	2.17	0.45
3:L:145:ALA:C	3:L:146:LEU:HD12	2.42	0.45
3:L:200:GLY:O	3:L:202:TYR:CE2	2.69	0.45
1:F:46:ASN:HA	1:F:112:ILE:O	2.17	0.44
1:F:155:GLY:O	1:F:156:HIS:C	2.60	0.44
2:G:50:LEU:HD22	2:G:124:TYR:HD2	1.82	0.44
1:I:123:TYR:N	1:I:138:LEU:O	2.49	0.44
1:I:218:SER:HA	1:I:233:VAL:HA	2.00	0.44
2:K:166:CYS:N	2:K:206:ALA:O	2.40	0.44
3:L:65:LEU:HD12	3:L:79:TYR:CD2	2.52	0.44
1:E:123:TYR:HE2	1:E:140:LEU:HD13	1.82	0.44
1:E:146:GLY:HA3	1:E:170:TRP:CD1	2.52	0.44
1:E:176:THR:CG2	1:E:219:CYS:SG	3.05	0.44
1:E:215:ARG:O	1:E:235:PHE:HA	2.18	0.44
2:G:63:MET:HG3	2:G:65:LEU:HB2	1.98	0.44
3:H:149:ASP:O	3:H:150:LEU:HD22	2.17	0.44
1:I:167:SER:O	1:I:202:MET:HE3	2.18	0.44
1:I:217:MET:C	1:I:234:ILE:HG22	2.42	0.44
1:J:31:ILE:HG22	1:J:32:VAL:N	2.32	0.44
1:J:148:LYS:HA	1:J:230:LYS:HE2	1.99	0.44
1:J:149:PRO:HD3	1:J:221:ILE:HG22	1.99	0.44
1:J:169:GLY:H	1:J:202:MET:HA	1.82	0.44
2:K:194:VAL:HA	2:K:203:GLU:O	2.17	0.44
1:E:47:THR:HB	1:E:112:ILE:HD12	2.00	0.44
1:E:153:MET:C	1:E:153:MET:SD	3.00	0.44
1:E:180:ASP:HB2	1:E:184:GLY:O	2.17	0.44
1:E:193:SER:HA	1:E:202:MET:O	2.18	0.44
1:E:223:ASN:CB	1:E:226:LEU:HB2	2.48	0.44
1:F:120:ASN:HA	1:F:142:VAL:HB	1.99	0.44
2:G:116:VAL:HG22	2:G:141:LEU:HD21	1.98	0.44
2:G:177:ILE:HD12	2:G:204:VAL:HG13	1.99	0.44
3:H:93:TYR:OH	3:H:120:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:162:ILE:HG22	3:H:163:HIS:N	2.31	0.44
1:J:67:PHE:HA	1:J:75:VAL:H	1.82	0.44
1:J:71:PHE:HZ	2:K:70:SER:HG	1.66	0.44
1:J:170:TRP:CE3	1:J:174:PRO:HB3	2.52	0.44
1:J:192:VAL:O	1:J:202:MET:O	2.35	0.44
1:E:153:MET:SD	1:F:235:PHE:HB3	2.57	0.44
1:E:171:TYR:CE1	1:E:172:PRO:HB3	2.53	0.44
1:F:153:MET:CB	1:F:163:LEU:HA	2.47	0.44
1:J:42:THR:CA	1:J:115:ILE:O	2.66	0.44
3:L:42:ALA:O	3:L:43:MET:HE2	2.17	0.44
1:E:147:SER:HB2	1:F:148:LYS:HE2	1.99	0.44
1:E:237:PRO:HG3	1:F:156:HIS:H	1.81	0.44
1:F:53:LEU:HG	1:F:103:ILE:HG13	2.00	0.44
1:F:117:ALA:O	1:F:171:TYR:CD1	2.70	0.44
1:F:177:VAL:HB	1:F:185:VAL:HG22	2.00	0.44
2:G:145:ALA:N	2:G:172:TYR:HB2	2.32	0.44
2:G:154:VAL:HG21	3:H:236:SER:H	1.82	0.44
3:H:165:GLU:HA	3:H:207:SER:HA	1.99	0.44
1:I:145:LEU:HD13	1:I:228:GLN:NE2	2.33	0.44
1:I:177:VAL:O	1:I:177:VAL:HG13	2.18	0.44
1:J:70:GLN:HB3	1:J:73:PRO:C	2.42	0.44
1:J:102:ASP:HB3	1:J:107:SER:O	2.18	0.44
2:K:96:ARG:HB3	2:K:114:HIS:HB2	1.99	0.44
3:L:175:PRO:HB3	3:L:224:SER:HA	2.00	0.44
1:E:153:MET:SD	1:F:236:ILE:N	2.91	0.44
1:E:155:GLY:H	1:E:162:ARG:HB3	1.82	0.44
1:E:170:TRP:HB2	1:E:203:VAL:H	1.83	0.44
1:E:235:PHE:O	1:F:153:MET:O	2.36	0.44
1:F:207:VAL:HG22	1:F:208:ILE:N	2.31	0.44
3:H:162:ILE:HG21	3:H:237:ILE:CD1	2.47	0.44
1:I:64:VAL:HG22	1:I:127:PHE:CE2	2.52	0.44
1:I:112:ILE:HG22	1:I:115:ILE:HD11	2.00	0.44
1:I:161:ILE:HD11	1:J:156:HIS:CD2	2.52	0.44
1:I:187:PRO:O	1:I:207:VAL:HG12	2.18	0.44
1:J:110:LEU:HG	1:J:112:ILE:CD1	2.47	0.44
3:L:91:ALA:HB3	3:L:92:PRO:HD3	1.99	0.44
3:L:93:TYR:CB	3:L:97:THR:HG23	2.48	0.44
3:L:154:VAL:HG22	3:L:155:LYS:N	2.31	0.44
3:L:181:ASN:O	3:L:184:GLY:N	2.46	0.44
3:L:203:ALA:O	3:L:204:VAL:HG13	2.18	0.44
1:E:177:VAL:HG22	1:E:222:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ASN:HD22	1:E:226:LEU:HD12	1.83	0.44
1:F:44:GLY:N	1:F:114:ASN:HA	2.33	0.44
1:F:74:ALA:O	1:F:88:GLN:NE2	2.45	0.44
1:F:179:ARG:N	1:F:218:SER:O	2.38	0.44
2:G:208:VAL:HG11	2:G:218:VAL:HG21	1.99	0.44
1:J:92:TYR:O	1:J:96:THR:HG23	2.18	0.44
3:L:39:PRO:CB	3:L:142:LYS:HB2	2.47	0.44
3:L:178:GLN:HG2	3:L:189:THR:HB	2.00	0.44
1:E:166:ILE:HG23	1:E:204:THR:OG1	2.17	0.44
1:E:239:SER:O	1:F:156:HIS:HB3	2.17	0.44
1:I:176:THR:HA	1:I:221:ILE:HA	2.00	0.44
1:J:53:LEU:HD13	1:J:57:LYS:CE	2.46	0.44
1:J:66:TRP:CD2	1:J:75:VAL:HG23	2.53	0.44
1:J:124:ARG:HD2	1:J:126:TYR:HH	1.83	0.44
2:K:235:ILE:HD12	3:L:235:ILE:HG23	2.00	0.44
3:L:169:THR:HA	3:L:203:ALA:HA	2.00	0.44
1:E:49:LEU:HD13	1:E:123:TYR:CD2	2.53	0.44
1:E:73:PRO:HB2	1:E:88:GLN:O	2.18	0.44
1:F:178:TRP:CE3	1:F:217:MET:HG3	2.52	0.44
1:F:220:SER:HA	1:F:230:LYS:O	2.18	0.44
1:F:235:PHE:C	1:F:236:ILE:HD13	2.42	0.44
2:G:104:ILE:O	2:G:105:THR:C	2.61	0.44
2:G:118:ALA:HB1	2:G:172:TYR:CZ	2.53	0.44
3:H:210:MET:HE3	3:H:217:GLY:HA2	1.99	0.44
1:J:194:MET:O	1:J:201:PHE:HA	2.17	0.44
2:K:224:ASN:O	2:K:228:GLY:N	2.51	0.44
3:L:76:VAL:CG2	3:L:111:LEU:HD21	2.47	0.44
3:L:177:ILE:HA	3:L:222:ILE:HA	1.99	0.44
3:L:223:ARG:HA	3:L:229:LEU:O	2.18	0.44
1:E:65:ARG:HD3	1:E:74:ALA:CB	2.48	0.43
1:E:153:MET:SD	1:F:235:PHE:C	3.01	0.43
2:G:167:ARG:HA	2:G:205:ALA:HA	2.00	0.43
1:I:216:ASN:HA	1:I:234:ILE:O	2.18	0.43
1:J:52:HIS:CB	1:J:107:SER:HA	2.47	0.43
1:J:66:TRP:CD1	1:J:125:CYS:SG	3.11	0.43
2:K:67:TRP:CD1	2:K:67:TRP:O	2.70	0.43
2:K:177:ILE:HG12	2:K:191:GLU:OE1	2.18	0.43
1:E:46:ASN:OD1	1:E:46:ASN:C	2.60	0.43
1:E:154:ARG:HE	1:E:164:GLU:CD	2.26	0.43
1:E:231:GLU:O	1:F:168:ARG:HD2	2.18	0.43
1:E:232:SER:HA	1:F:150:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:GLN:NE2	1:F:230:LYS:HD2	2.34	0.43
2:G:51:PRO:HA	2:G:111:LEU:H	1.83	0.43
1:I:221:ILE:O	1:I:228:GLN:O	2.36	0.43
1:J:65:ARG:O	1:J:127:PHE:HA	2.17	0.43
2:K:50:LEU:HD13	2:K:124:TYR:CE2	2.53	0.43
3:L:70:SER:HB2	3:L:123:LYS:HB3	1.99	0.43
3:L:87:ASP:OD1	3:L:88:ARG:NH1	2.51	0.43
1:E:74:ALA:C	1:E:89:MET:H	2.22	0.43
1:E:95:ARG:HD2	1:E:114:ASN:HB3	1.99	0.43
2:G:76:VAL:HB	2:G:111:LEU:HD11	2.01	0.43
2:G:169:THR:HA	2:G:203:GLU:HA	1.99	0.43
1:J:129:GLU:HG2	2:K:131:GLY:N	2.34	0.43
1:J:191:GLU:HA	1:J:204:THR:HG23	2.00	0.43
3:L:180:SER:OG	3:L:221:THR:HB	2.18	0.43
1:E:61:ASP:CB	1:E:80:GLY:H	2.31	0.43
1:E:217:MET:H	1:E:234:ILE:HG23	1.84	0.43
1:F:42:THR:HG22	1:F:43:VAL:HG12	2.00	0.43
1:I:115:ILE:HD13	1:I:119:GLU:HG2	2.00	0.43
2:K:65:LEU:HD21	2:K:67:TRP:HB2	2.00	0.43
2:K:179:TRP:CD1	2:K:189:ALA:HB3	2.53	0.43
3:L:43:MET:C	3:L:143:VAL:HG13	2.43	0.43
1:E:144:GLY:H	1:E:171:TYR:HB3	1.82	0.43
1:F:217:MET:O	1:F:233:VAL:HA	2.18	0.43
1:F:221:ILE:HD12	1:F:230:LYS:HD2	2.00	0.43
2:G:49:ASP:C	2:G:50:LEU:HD12	2.44	0.43
2:G:146:LEU:CD2	2:G:229:LEU:HD12	2.46	0.43
3:H:191:GLU:HA	3:H:205:ALA:O	2.19	0.43
1:I:149:PRO:HD3	1:I:230:LYS:O	2.18	0.43
1:I:152:SER:O	1:I:164:GLU:O	2.35	0.43
1:I:167:SER:O	1:I:202:MET:HB2	2.18	0.43
2:K:56:PRO:HG2	2:K:128:PHE:CZ	2.53	0.43
3:L:80:ALA:HB2	3:L:85:VAL:CG1	2.48	0.43
1:E:153:MET:C	1:F:235:PHE:HB3	2.42	0.43
1:E:156:HIS:HB2	1:F:237:PRO:CG	2.48	0.43
1:E:174:PRO:HG3	1:E:223:ASN:CG	2.44	0.43
1:F:43:VAL:N	1:F:116:THR:HA	2.33	0.43
1:F:160:GLY:O	1:F:161:ILE:CG2	2.66	0.43
1:F:221:ILE:HB	1:F:230:LYS:HB2	2.01	0.43
2:G:172:TYR:HA	2:G:202:TYR:HE2	1.84	0.43
3:H:221:THR:HG22	3:H:232:THR:HA	1.99	0.43
1:I:164:GLU:HA	1:I:205:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:THR:OG1	1:I:206:ALA:N	2.51	0.43
1:J:49:LEU:HB3	1:J:66:TRP:HH2	1.82	0.43
1:J:66:TRP:HE3	1:J:76:PHE:HB3	1.83	0.43
2:K:179:TRP:CD1	2:K:206:ALA:HB1	2.53	0.43
3:L:102:ASP:OD1	3:L:103:GLY:N	2.46	0.43
3:L:137:ALA:O	3:L:138:LEU:HG	2.18	0.43
1:E:66:TRP:CH2	1:E:78:TYR:CE2	3.06	0.43
1:E:92:TYR:OH	1:E:119:GLU:HB3	2.19	0.43
1:E:177:VAL:HG21	1:E:229:LYS:CE	2.48	0.43
1:F:151:ILE:HD12	1:F:178:TRP:CZ3	2.52	0.43
1:F:240:PHE:N	1:F:240:PHE:CD1	2.86	0.43
2:G:69:SER:O	2:G:70:SER:C	2.62	0.43
1:J:163:LEU:C	1:J:164:GLU:HG3	2.44	0.43
2:K:146:LEU:HA	2:K:224:ASN:HB2	1.99	0.43
2:K:179:TRP:N	2:K:188:PRO:HA	2.33	0.43
2:K:191:GLU:OE1	2:K:206:ALA:HB2	2.19	0.43
2:K:197:ASP:O	2:K:200:GLY:N	2.47	0.43
3:L:33:VAL:HG12	3:L:52:CYS:HB3	1.99	0.43
3:L:175:PRO:HB2	3:L:222:ILE:HG22	2.00	0.43
1:E:162:ARG:NH2	1:E:206:ALA:HB1	2.33	0.43
1:F:170:TRP:CD2	1:F:174:PRO:HB3	2.54	0.43
1:F:180:ASP:HB3	1:F:217:MET:HA	2.01	0.43
2:G:178:GLN:HG3	2:G:187:ILE:CG2	2.48	0.43
1:I:152:SER:C	1:I:164:GLU:HB2	2.43	0.43
1:J:51:CYS:O	1:J:108:VAL:N	2.52	0.43
3:L:116:VAL:HG21	3:L:141:LEU:HD13	2.01	0.43
3:L:204:VAL:HG11	3:L:222:ILE:HG23	2.00	0.43
1:E:57:LYS:HZ2	1:E:59:ALA:CB	2.31	0.43
1:E:60:GLU:HB2	1:E:81:GLY:HA2	1.99	0.43
1:E:64:VAL:HG12	1:E:126:TYR:CE2	2.54	0.43
1:E:145:LEU:HD13	1:E:228:GLN:HG2	2.01	0.43
1:E:151:ILE:HD11	1:E:232:SER:O	2.19	0.43
1:E:165:CYS:H	1:E:205:THR:CG2	2.31	0.43
1:E:231:GLU:O	1:F:150:LEU:HD11	2.19	0.43
1:F:47:THR:HG23	1:F:140:LEU:HD13	1.99	0.43
2:G:44:VAL:HA	2:G:117:THR:HA	2.00	0.43
1:I:153:MET:O	1:J:235:PHE:HB3	2.19	0.43
1:I:170:TRP:CE3	1:I:174:PRO:HG3	2.54	0.43
1:J:148:LYS:HD2	1:J:230:LYS:HB3	2.00	0.43
1:J:186:ALA:HB2	1:J:217:MET:HE1	2.01	0.43
1:J:213:SER:OG	1:J:214:VAL:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:PRO:HA	2:K:140:GLU:HB3	2.00	0.43
3:L:146:LEU:HA	3:L:171:TRP:CE3	2.54	0.43
1:E:66:TRP:CE3	1:E:76:PHE:O	2.72	0.43
1:E:67:PHE:HZ	1:E:135:GLU:OE2	2.02	0.43
1:E:149:PRO:HB3	1:E:219:CYS:SG	2.59	0.43
1:E:150:LEU:HD11	1:E:168:ARG:HH11	1.83	0.43
1:E:153:MET:CE	1:E:155:GLY:N	2.82	0.43
1:E:234:ILE:O	1:E:236:ILE:HG13	2.17	0.43
1:F:58:ASN:O	1:F:78:TYR:OH	2.37	0.43
1:F:69:SER:HB3	1:F:124:ARG:H	1.84	0.43
1:F:153:MET:O	1:F:164:GLU:OE2	2.37	0.43
3:H:125:LEU:HD13	3:H:137:ALA:O	2.19	0.43
1:I:149:PRO:CD	1:I:230:LYS:O	2.67	0.43
1:I:157:GLU:O	1:I:160:GLY:N	2.51	0.43
1:I:193:SER:OG	1:I:201:PHE:HB3	2.19	0.43
1:J:52:HIS:HA	1:J:106:GLY:O	2.18	0.43
1:J:149:PRO:HD3	1:J:230:LYS:HB3	2.00	0.43
2:K:75:VAL:HG11	2:K:88:ARG:O	2.19	0.43
3:L:54:LEU:CD2	3:L:130:ASP:OD2	2.67	0.43
1:E:64:VAL:HG21	1:E:127:PHE:HA	2.01	0.42
1:E:152:SER:O	1:E:163:LEU:HA	2.19	0.42
1:E:213:SER:HA	1:E:238:GLU:HA	2.01	0.42
1:F:54:SER:OG	1:F:55:PRO:HD3	2.19	0.42
1:F:150:LEU:HD11	1:F:168:ARG:CD	2.49	0.42
1:F:151:ILE:HG23	1:F:178:TRP:CH2	2.54	0.42
3:H:169:THR:HA	3:H:203:ALA:HA	2.01	0.42
3:H:177:ILE:HG23	3:H:189:THR:HG22	1.99	0.42
3:H:189:THR:OG1	3:H:206:ALA:HB2	2.19	0.42
1:I:112:ILE:HD13	1:I:123:TYR:CE2	2.53	0.42
1:J:150:LEU:HD11	1:J:166:ILE:CD1	2.48	0.42
1:E:43:VAL:O	1:E:44:GLY:C	2.63	0.42
1:F:46:ASN:HD21	1:F:113:HIS:CG	2.37	0.42
1:F:91:GLU:CB	1:F:116:THR:HB	2.48	0.42
1:F:149:PRO:HG2	1:F:231:GLU:O	2.19	0.42
2:G:171:TRP:HB2	2:G:175:PRO:HD3	2.01	0.42
2:G:190:VAL:O	2:G:190:VAL:HG13	2.18	0.42
1:J:67:PHE:HB2	1:J:70:GLN:OE1	2.19	0.42
3:L:65:LEU:HA	3:L:128:PHE:CE1	2.54	0.42
3:L:204:VAL:HG21	3:L:222:ILE:CD1	2.49	0.42
1:E:67:PHE:N	1:E:75:VAL:HG22	2.34	0.42
1:E:75:VAL:O	1:E:76:PHE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:VAL:HG21	1:E:108:VAL:HA	2.00	0.42
1:E:172:PRO:HA	1:E:201:PHE:HB2	2.01	0.42
1:E:176:THR:HA	1:E:220:SER:O	2.19	0.42
1:F:154:ARG:CG	1:F:190:LYS:HD3	2.49	0.42
1:F:177:VAL:HG22	1:F:220:SER:O	2.18	0.42
1:F:182:TYR:CE1	1:F:214:VAL:HG23	2.54	0.42
1:F:189:LEU:C	1:F:189:LEU:HD12	2.44	0.42
2:G:118:ALA:HB1	2:G:172:TYR:OH	2.19	0.42
2:G:140:GLU:OE2	2:G:142:LYS:HB3	2.18	0.42
2:G:178:GLN:CB	2:G:187:ILE:O	2.67	0.42
2:G:179:TRP:HE1	2:G:206:ALA:HB3	1.84	0.42
2:G:187:ILE:O	2:G:187:ILE:HG23	2.19	0.42
1:I:42:THR:O	1:I:43:VAL:C	2.62	0.42
1:I:153:MET:HE3	1:I:156:HIS:CE1	2.54	0.42
1:J:77:VAL:HG12	1:J:78:TYR:N	2.33	0.42
1:J:116:THR:CG2	1:J:118:GLN:HG2	2.49	0.42
2:K:43:MET:HE3	2:K:145:ALA:HA	2.02	0.42
3:L:124:TYR:CE1	3:L:141:LEU:HD12	2.54	0.42
3:L:235:ILE:HG22	3:L:236:SER:H	1.84	0.42
1:E:139:HIS:ND1	1:E:140:LEU:N	2.67	0.42
1:F:91:GLU:O	1:F:114:ASN:CG	2.63	0.42
2:G:178:GLN:O	2:G:221:ILE:N	2.42	0.42
2:G:180:SER:O	2:G:219:SER:HB3	2.19	0.42
1:I:147:SER:H	1:I:167:SER:HB3	1.83	0.42
1:I:217:MET:H	1:I:234:ILE:CG2	2.31	0.42
1:J:35:PRO:HD2	1:J:138:LEU:HD13	2.01	0.42
1:J:150:LEU:CG	1:J:166:ILE:HB	2.49	0.42
2:K:103:GLY:O	2:K:106:ALA:N	2.52	0.42
1:E:61:ASP:HA	1:E:79:LYS:HA	2.01	0.42
1:E:67:PHE:O	1:E:67:PHE:CG	2.72	0.42
1:E:196:ASP:O	1:E:197:ALA:C	2.61	0.42
1:F:41:ALA:CB	1:F:115:ILE:HB	2.49	0.42
1:F:77:VAL:HG21	1:F:87:GLU:HB2	2.02	0.42
1:I:176:THR:OG1	1:I:221:ILE:HG12	2.20	0.42
1:I:214:VAL:HG22	1:I:217:MET:CE	2.50	0.42
1:J:42:THR:HG22	1:J:43:VAL:N	2.35	0.42
1:J:42:THR:N	1:J:45:GLU:HB2	2.34	0.42
1:J:241:MET:HE3	1:J:242:PRO:O	2.19	0.42
2:K:32:SER:OG	2:K:33:VAL:N	2.53	0.42
2:K:171:TRP:HZ3	2:K:224:ASN:HB2	1.83	0.42
2:K:221:ILE:HA	2:K:231:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:197:ASP:OD1	3:L:201:LEU:HB2	2.19	0.42
1:E:74:ALA:HB3	1:E:77:VAL:CG2	2.50	0.42
1:E:78:TYR:HB2	1:E:82:ARG:O	2.20	0.42
1:E:147:SER:O	1:E:167:SER:OG	2.37	0.42
1:E:192:VAL:O	1:E:203:VAL:HA	2.19	0.42
1:F:38:PRO:O	1:F:40:LEU:HD22	2.20	0.42
1:F:128:GLN:O	1:F:128:GLN:HG2	2.18	0.42
1:F:215:ARG:NH2	1:F:238:GLU:HG2	2.35	0.42
1:F:223:ASN:HB2	1:F:227:GLY:H	1.84	0.42
2:G:222:ILE:O	2:G:230:GLU:CB	2.68	0.42
1:I:148:LYS:CB	1:J:150:LEU:HB3	2.49	0.42
1:J:91:GLU:OE2	1:J:198:ASP:CG	2.63	0.42
1:J:175:LEU:HB3	1:J:222:ASN:OD1	2.20	0.42
1:J:215:ARG:NE	1:J:215:ARG:HA	2.34	0.42
2:K:179:TRP:HB2	2:K:189:ALA:N	2.34	0.42
3:L:121:SER:OG	3:L:172:TYR:OH	2.29	0.42
1:E:192:VAL:O	1:E:192:VAL:HG13	2.19	0.42
1:E:237:PRO:HB3	1:F:154:ARG:O	2.20	0.42
1:F:42:THR:HG22	1:F:43:VAL:H	1.83	0.42
1:F:51:CYS:O	1:F:108:VAL:HG22	2.20	0.42
1:F:55:PRO:O	1:F:57:LYS:HG2	2.20	0.42
2:G:232:THR:HG22	2:G:233:ALA:N	2.35	0.42
3:H:238:ALA:HB1	3:H:240:PRO:HD2	2.01	0.42
1:I:148:LYS:N	1:I:230:LYS:HE3	2.35	0.42
1:I:234:ILE:CG1	1:J:153:MET:SD	3.08	0.42
1:J:42:THR:H	1:J:45:GLU:HB2	1.83	0.42
1:J:67:PHE:CA	1:J:75:VAL:HG22	2.48	0.42
1:J:146:GLY:HA3	1:J:170:TRP:CD1	2.54	0.42
2:K:176:GLN:N	2:K:223:ARG:O	2.39	0.42
3:L:237:ILE:HG22	3:L:238:ALA:N	2.33	0.42
1:E:74:ALA:C	1:E:89:MET:HB2	2.45	0.42
1:E:147:SER:C	1:E:167:SER:OG	2.63	0.42
1:E:148:LYS:C	1:F:150:LEU:HD21	2.45	0.42
1:E:180:ASP:OD1	1:E:181:PRO:HD2	2.20	0.42
1:E:234:ILE:O	1:E:234:ILE:CG2	2.66	0.42
1:F:54:SER:O	1:F:103:ILE:O	2.38	0.42
1:F:214:VAL:HG22	1:F:215:ARG:N	2.35	0.42
2:G:177:ILE:HG13	2:G:222:ILE:HG13	2.01	0.42
2:G:207:SER:OG	2:G:208:VAL:N	2.53	0.42
1:I:176:THR:HG21	1:I:205:THR:HG21	2.02	0.42
1:J:66:TRP:CD1	1:J:125:CYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:VAL:N	1:J:220:SER:O	2.52	0.42
2:K:180:SER:C	2:K:219:SER:O	2.63	0.42
3:L:171:TRP:HB3	3:L:175:PRO:CG	2.49	0.42
1:E:99:VAL:HG21	1:E:102:ASP:OD2	2.19	0.42
1:E:163:LEU:HD13	1:E:209:ILE:HG13	2.02	0.42
1:E:171:TYR:HD2	1:E:201:PHE:H	1.67	0.42
1:F:49:LEU:HB2	1:F:110:LEU:HB3	2.01	0.42
1:F:57:LYS:HB3	2:G:130:ASP:HA	2.02	0.42
1:F:216:ASN:OD1	1:F:235:PHE:HD1	2.03	0.42
2:G:165:GLU:HA	2:G:207:SER:HA	2.01	0.42
3:H:48:ALA:HB3	3:H:113:ILE:HB	2.01	0.42
1:J:149:PRO:HG3	1:J:221:ILE:CG2	2.49	0.42
2:K:171:TRP:O	2:K:200:GLY:O	2.38	0.42
2:K:194:VAL:HA	2:K:203:GLU:C	2.45	0.42
3:L:93:TYR:HB3	3:L:96:ARG:HB2	2.02	0.42
1:E:59:ALA:CB	1:E:62:MET:HB2	2.49	0.42
1:F:215:ARG:O	1:F:235:PHE:HA	2.20	0.42
1:F:217:MET:CB	1:F:234:ILE:O	2.68	0.42
2:G:32:SER:HA	2:G:133:PHE:CZ	2.55	0.42
1:I:43:VAL:HG22	1:I:200:LEU:HD21	2.01	0.42
1:I:151:ILE:O	1:J:234:ILE:HB	2.20	0.42
1:J:97:THR:N	1:J:111:VAL:O	2.53	0.42
1:J:139:HIS:CG	1:J:140:LEU:N	2.88	0.42
1:J:221:ILE:N	1:J:230:LYS:O	2.44	0.42
2:K:49:ASP:C	2:K:50:LEU:HD23	2.45	0.42
3:L:237:ILE:CG2	3:L:238:ALA:N	2.82	0.42
1:E:30:PHE:CZ	1:E:57:LYS:HE2	2.55	0.41
1:F:171:TYR:CD1	1:F:171:TYR:C	2.98	0.41
1:F:179:ARG:HD3	1:F:220:SER:OG	2.20	0.41
2:G:112:ARG:O	2:G:113:ILE:HD13	2.20	0.41
2:G:177:ILE:HA	2:G:222:ILE:HA	2.02	0.41
3:H:67:TRP:NE1	3:H:99:ILE:HD12	2.34	0.41
3:H:178:GLN:N	3:H:221:THR:O	2.43	0.41
1:I:42:THR:O	1:I:115:ILE:O	2.38	0.41
1:I:170:TRP:HB3	1:I:174:PRO:HG3	2.02	0.41
1:J:43:VAL:CB	1:J:200:LEU:HD11	2.48	0.41
1:J:56:GLU:OE1	1:J:56:GLU:HA	2.20	0.41
1:J:61:ASP:O	1:J:62:MET:HG2	2.20	0.41
1:J:66:TRP:HE3	1:J:76:PHE:CB	2.33	0.41
1:J:116:THR:OG1	1:J:199:GLY:O	2.37	0.41
1:J:129:GLU:CD	2:K:131:GLY:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:179:TRP:O	2:K:187:ILE:C	2.63	0.41
1:E:45:GLU:O	1:E:115:ILE:HG12	2.20	0.41
1:E:89:MET:HE3	1:E:91:GLU:HB3	2.02	0.41
1:E:147:SER:HA	1:F:148:LYS:CB	2.50	0.41
1:E:150:LEU:HB3	1:F:233:VAL:H	1.85	0.41
1:E:153:MET:HE3	1:F:237:PRO:CD	2.50	0.41
1:E:188:ALA:HA	1:E:207:VAL:CG1	2.44	0.41
1:E:214:VAL:C	1:E:236:ILE:HB	2.45	0.41
1:F:65:ARG:HE	1:F:67:PHE:HD2	1.68	0.41
2:G:33:VAL:HG13	2:G:51:PRO:O	2.19	0.41
2:G:45:GLY:N	2:G:116:VAL:O	2.36	0.41
2:G:144:ALA:HB2	2:G:226:LEU:HD23	2.01	0.41
1:J:46:ASN:OD1	1:J:111:VAL:HG12	2.20	0.41
1:J:150:LEU:HD12	1:J:151:ILE:CA	2.50	0.41
2:K:223:ARG:HE	2:K:225:SER:HA	1.86	0.41
3:L:68:VAL:HB	3:L:125:LEU:HB2	2.01	0.41
3:L:232:THR:HG22	3:L:233:ALA:N	2.35	0.41
1:E:64:VAL:HB	1:E:126:TYR:CE2	2.55	0.41
1:E:148:LYS:H	1:F:148:LYS:HB2	1.84	0.41
1:E:167:SER:OG	1:E:221:ILE:HD12	2.20	0.41
1:F:68:ARG:HE	1:F:75:VAL:HG11	1.85	0.41
1:F:170:TRP:CE2	1:F:174:PRO:HB3	2.55	0.41
1:F:189:LEU:N	1:F:206:ALA:HB3	2.32	0.41
3:H:157:TYR:O	3:H:244:SER:OG	2.31	0.41
3:H:162:ILE:HG13	3:H:237:ILE:HD12	2.02	0.41
3:H:178:GLN:HG3	3:H:187:ILE:C	2.46	0.41
2:K:133:PHE:O	2:K:134:TYR:HB3	2.20	0.41
2:K:178:GLN:NE2	2:K:186:ASN:OD1	2.47	0.41
1:E:64:VAL:CG1	1:E:128:GLN:HG2	2.51	0.41
1:E:92:TYR:CE1	1:E:119:GLU:HG2	2.55	0.41
1:E:98:PHE:HA	1:E:109:ALA:O	2.20	0.41
1:E:117:ALA:HA	1:E:142:VAL:HG11	2.01	0.41
1:E:151:ILE:CG2	1:E:234:ILE:HD12	2.50	0.41
1:E:213:SER:HA	1:E:237:PRO:O	2.21	0.41
1:F:151:ILE:HA	1:F:165:CYS:HA	2.02	0.41
1:F:162:ARG:CB	1:F:208:ILE:HA	2.50	0.41
2:G:200:GLY:O	2:G:201:LEU:HG	2.20	0.41
3:H:66:LYS:NZ	3:H:75:VAL:HG13	2.35	0.41
3:H:67:TRP:CZ3	3:H:126:CYS:SG	3.14	0.41
3:H:143:VAL:HG12	3:H:144:ALA:N	2.34	0.41
1:I:134:ASP:OD1	1:I:134:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:GLY:CA	1:J:237:PRO:HG2	2.51	0.41
1:J:59:ALA:HB3	1:J:103:ILE:HD13	2.03	0.41
1:J:167:SER:HB2	1:J:221:ILE:HD13	2.02	0.41
2:K:52:CYS:HB2	2:K:67:TRP:HH2	1.85	0.41
2:K:118:ALA:C	2:K:199:VAL:O	2.63	0.41
3:L:148:SER:C	3:L:168:SER:HB2	2.45	0.41
1:E:66:TRP:CE2	1:E:108:VAL:HG21	2.56	0.41
1:E:147:SER:N	1:E:167:SER:HB3	2.35	0.41
1:E:155:GLY:C	1:F:237:PRO:HB3	2.46	0.41
1:E:188:ALA:CB	1:E:207:VAL:HG12	2.50	0.41
1:E:216:ASN:C	1:E:236:ILE:HD12	2.44	0.41
1:E:235:PHE:O	1:F:153:MET:C	2.64	0.41
1:I:102:ASP:O	1:I:105:ARG:NH1	2.54	0.41
1:I:149:PRO:HG3	1:I:221:ILE:CG1	2.50	0.41
2:K:208:VAL:HG11	2:K:218:VAL:HG13	2.02	0.41
3:L:84:GLU:HB2	3:L:99:ILE:O	2.20	0.41
3:L:218:VAL:HG22	3:L:219:SER:N	2.35	0.41
1:E:64:VAL:CG2	1:E:128:GLN:HG2	2.50	0.41
1:E:79:LYS:HD2	1:E:80:GLY:N	2.36	0.41
1:E:155:GLY:O	1:E:161:ILE:HA	2.20	0.41
1:E:177:VAL:HG23	1:E:177:VAL:O	2.19	0.41
1:E:191:GLU:HG3	1:E:203:VAL:HG13	2.02	0.41
1:F:150:LEU:HA	1:F:150:LEU:HD23	1.74	0.41
3:H:113:ILE:HD13	3:H:124:TYR:CZ	2.56	0.41
3:H:164:LEU:HD21	3:H:208:VAL:CG1	2.50	0.41
3:H:185:GLU:HG3	3:H:186:ASN:H	1.85	0.41
1:I:150:LEU:HB3	1:J:233:VAL:H	1.86	0.41
1:I:152:SER:O	1:I:164:GLU:N	2.50	0.41
1:J:61:ASP:HA	1:J:78:TYR:CE1	2.56	0.41
1:J:74:ALA:O	1:J:88:GLN:HA	2.20	0.41
2:K:147:GLY:CA	2:K:171:TRP:CE2	3.04	0.41
3:L:121:SER:CB	3:L:143:VAL:H	2.32	0.41
1:E:66:TRP:HA	1:E:125:CYS:HA	2.02	0.41
1:E:74:ALA:C	1:E:89:MET:N	2.79	0.41
1:E:152:SER:HA	1:F:234:ILE:HG13	2.02	0.41
1:E:211:ASP:OD1	1:E:212:LYS:N	2.44	0.41
1:I:44:GLY:H	1:I:116:THR:HA	1.86	0.41
1:I:150:LEU:HB2	1:I:166:ILE:HB	2.03	0.41
2:K:197:ASP:OD2	2:K:201:LEU:HB2	2.20	0.41
1:E:102:ASP:HB2	1:E:108:VAL:HG12	2.02	0.41
1:E:149:PRO:HA	1:E:221:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:HG	1:E:166:ILE:O	2.19	0.41
1:F:41:ALA:HB1	1:F:115:ILE:HB	2.01	0.41
2:G:44:VAL:HG13	2:G:117:THR:HG22	2.03	0.41
2:G:194:VAL:HA	2:G:203:GLU:O	2.21	0.41
1:I:235:PHE:O	1:I:236:ILE:HG13	2.21	0.41
1:J:41:ALA:HB2	1:J:47:THR:OG1	2.20	0.41
1:J:66:TRP:HA	1:J:126:TYR:O	2.21	0.41
1:J:125:CYS:SG	1:J:127:PHE:CD1	3.13	0.41
3:L:50:LEU:N	3:L:111:LEU:O	2.46	0.41
1:E:46:ASN:OD1	1:E:111:VAL:CG1	2.69	0.41
1:E:92:TYR:OH	1:E:123:TYR:OH	2.24	0.41
1:E:112:ILE:CG2	1:E:113:HIS:N	2.84	0.41
1:E:120:ASN:ND2	1:E:141:VAL:HG23	2.35	0.41
1:E:126:TYR:HD2	1:E:133:TYR:CG	2.39	0.41
1:E:154:ARG:HG2	1:E:162:ARG:NH1	2.36	0.41
1:E:168:ARG:HH12	1:F:149:PRO:CG	2.34	0.41
1:E:173:LYS:O	1:E:224:THR:OG1	2.32	0.41
1:E:176:THR:HB	1:E:191:GLU:OE1	2.19	0.41
1:F:52:HIS:CD2	1:F:106:GLY:O	2.74	0.41
1:F:67:PHE:CD1	1:F:70:GLN:O	2.74	0.41
1:F:89:MET:HE3	1:F:90:GLU:HG3	2.03	0.41
1:F:174:PRO:HB2	1:F:221:ILE:HG23	2.03	0.41
2:G:187:ILE:O	2:G:188:PRO:C	2.64	0.41
3:H:44:VAL:HG22	3:H:118:ALA:N	2.36	0.41
3:H:89:GLN:OE1	3:H:97:THR:OG1	2.39	0.41
1:I:145:LEU:HD22	1:I:228:GLN:CD	2.46	0.41
1:I:152:SER:HA	1:J:234:ILE:CG1	2.51	0.41
1:J:74:ALA:HB3	1:J:77:VAL:HG23	2.03	0.41
1:J:172:PRO:HA	1:J:201:PHE:CD2	2.56	0.41
1:J:177:VAL:O	1:J:219:CYS:HA	2.21	0.41
1:J:186:ALA:CB	1:J:217:MET:HE1	2.51	0.41
1:J:194:MET:HE1	1:J:196:ASP:HA	2.02	0.41
2:K:50:LEU:HD13	2:K:124:TYR:CE1	2.56	0.41
2:K:157:TYR:CD2	3:L:240:PRO:HG2	2.56	0.41
2:K:176:GLN:OE1	2:K:224:ASN:HA	2.20	0.41
3:L:162:ILE:HG22	3:L:163:HIS:H	1.86	0.41
1:E:66:TRP:CD1	1:E:110:LEU:HD22	2.56	0.41
1:E:162:ARG:NH1	1:E:164:GLU:HB3	2.36	0.41
1:E:163:LEU:HB2	1:E:207:VAL:CG2	2.51	0.41
1:E:181:PRO:CD	1:E:216:ASN:HB2	2.50	0.41
1:E:214:VAL:HG12	1:E:215:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:PRO:O	1:F:173:LYS:HG3	2.21	0.41
1:F:181:PRO:O	1:F:182:TYR:HD1	2.04	0.41
2:G:89:GLN:OE1	2:G:94:ARG:NH1	2.54	0.41
1:I:153:MET:SD	1:J:237:PRO:HD2	2.60	0.41
1:I:241:MET:HE3	1:I:242:PRO:O	2.21	0.41
1:J:124:ARG:HD2	1:J:135:GLU:OE2	2.21	0.41
1:J:201:PHE:O	1:J:203:VAL:HG13	2.21	0.41
2:K:164:LEU:HD12	2:K:210:MET:CE	2.51	0.41
3:L:171:TRP:CE2	3:L:222:ILE:HG21	2.56	0.41
1:E:215:ARG:NH2	1:E:237:PRO:O	2.54	0.40
1:E:216:ASN:OD1	1:E:235:PHE:HA	2.22	0.40
1:F:222:ASN:O	1:F:223:ASN:CG	2.64	0.40
2:G:92:PRO:O	2:G:96:ARG:NE	2.54	0.40
3:H:178:GLN:HG2	3:H:186:ASN:HA	2.01	0.40
1:I:41:ALA:CB	1:I:142:VAL:HG22	2.51	0.40
1:J:40:LEU:HD13	1:J:141:VAL:C	2.46	0.40
1:J:48:THR:CA	1:J:111:VAL:HG22	2.46	0.40
1:J:73:PRO:HA	1:J:87:GLU:HB3	2.03	0.40
2:K:149:ASN:HB3	2:K:169:THR:HG23	2.02	0.40
3:L:33:VAL:HG21	3:L:128:PHE:CD1	2.56	0.40
3:L:173:PRO:O	3:L:202:TYR:CG	2.75	0.40
1:E:45:GLU:H	1:E:115:ILE:HB	1.87	0.40
1:E:78:TYR:CD1	1:E:78:TYR:C	2.99	0.40
1:E:171:TYR:CD1	1:E:172:PRO:N	2.89	0.40
1:F:67:PHE:CZ	1:F:71:PHE:CD1	3.09	0.40
1:F:175:LEU:HB3	1:F:177:VAL:HG13	2.03	0.40
2:G:64:GLU:CD	2:G:65:LEU:N	2.79	0.40
2:G:196:ALA:HA	2:G:201:LEU:H	1.86	0.40
3:H:149:ASP:O	3:H:167:ARG:O	2.39	0.40
3:H:170:GLY:C	3:H:201:LEU:HB3	2.46	0.40
1:I:123:TYR:CD1	1:I:140:LEU:HD13	2.56	0.40
1:I:155:GLY:CA	1:I:162:ARG:HB3	2.51	0.40
1:J:71:PHE:C	1:J:73:PRO:HD2	2.46	0.40
1:J:91:GLU:HB3	1:J:114:ASN:CG	2.46	0.40
1:J:115:ILE:CG2	1:J:123:TYR:OH	2.70	0.40
1:J:117:ALA:CB	1:J:144:GLY:HA2	2.50	0.40
1:J:163:LEU:HB2	1:J:207:VAL:HG13	2.03	0.40
2:K:31:PHE:HB2	2:K:55:PHE:H	1.86	0.40
2:K:146:LEU:HD12	2:K:147:GLY:H	1.86	0.40
2:K:171:TRP:CG	2:K:175:PRO:HD3	2.56	0.40
1:E:38:PRO:HA	1:E:139:HIS:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LYS:HD2	1:E:128:GLN:O	2.20	0.40
1:E:64:VAL:CG1	1:E:126:TYR:CE2	3.05	0.40
1:E:78:TYR:O	3:L:134:TYR:OH	2.27	0.40
1:E:198:ASP:OD1	1:E:200:LEU:HB2	2.21	0.40
1:E:240:PHE:CE2	1:F:156:HIS:CG	3.09	0.40
1:F:151:ILE:HG23	1:F:178:TRP:HH2	1.86	0.40
3:H:118:ALA:HB1	3:H:172:TYR:CG	2.56	0.40
1:I:189:LEU:HD11	1:I:208:ILE:HB	2.03	0.40
1:J:176:THR:HB	1:J:205:THR:HG21	2.02	0.40
3:L:121:SER:O	3:L:141:LEU:O	2.40	0.40
1:E:148:LYS:H	1:F:148:LYS:CB	2.35	0.40
1:E:170:TRP:CZ2	1:E:221:ILE:O	2.75	0.40
1:E:190:LYS:N	1:E:206:ALA:O	2.50	0.40
1:F:77:VAL:HB	1:F:84:ARG:HB2	2.04	0.40
2:G:39:PRO:HA	2:G:140:GLU:HB3	2.03	0.40
2:G:174:GLN:CD	2:G:175:PRO:HD2	2.47	0.40
3:H:31:PHE:HB2	3:H:54:LEU:HD23	2.04	0.40
1:I:75:VAL:HG11	1:I:110:LEU:HD21	2.03	0.40
1:I:148:LYS:O	1:J:149:PRO:O	2.39	0.40
1:J:40:LEU:HD12	1:J:143:ALA:N	2.37	0.40
1:J:143:ALA:HA	1:J:225:LEU:HD22	2.03	0.40
1:J:166:ILE:CG1	1:J:204:THR:OG1	2.70	0.40
1:J:174:PRO:HB3	1:J:223:ASN:HA	2.03	0.40
2:K:113:ILE:HD12	2:K:141:LEU:HD13	2.03	0.40
2:K:171:TRP:O	2:K:201:LEU:HA	2.21	0.40
3:L:54:LEU:HD22	3:L:58:MET:HB2	2.04	0.40
3:L:64:GLU:N	3:L:81:ASP:OD1	2.55	0.40
1:E:50:ARG:HH11	1:E:109:ALA:N	2.19	0.40
1:E:66:TRP:HA	1:E:125:CYS:CB	2.51	0.40
1:E:126:TYR:HB2	1:E:133:TYR:CD1	2.56	0.40
1:E:152:SER:HB3	1:E:164:GLU:O	2.22	0.40
1:F:51:CYS:HB3	1:F:108:VAL:HG23	2.02	0.40
2:G:102:ASP:OD1	2:G:102:ASP:N	2.55	0.40
2:G:179:TRP:O	2:G:180:SER:OG	2.33	0.40
3:H:121:SER:OG	3:H:143:VAL:HG23	2.22	0.40
1:I:220:SER:HA	1:I:231:GLU:HA	2.04	0.40
1:I:235:PHE:C	1:I:236:ILE:HG13	2.45	0.40
2:K:152:VAL:HG12	2:K:153:GLU:N	2.35	0.40
2:K:172:TYR:HA	2:K:174:GLN:N	2.37	0.40
3:L:85:VAL:HG21	3:L:88:ARG:HD2	2.04	0.40
3:L:177:ILE:HG23	3:L:191:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:TRP:CE3	3:L:218:VAL:HG13	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	214/534 (40%)	159 (74%)	55 (26%)	0	100	100
1	F	214/534 (40%)	155 (72%)	59 (28%)	0	100	100
1	I	214/534 (40%)	178 (83%)	36 (17%)	0	100	100
1	J	214/534 (40%)	159 (74%)	55 (26%)	0	100	100
2	G	214/340 (63%)	160 (75%)	53 (25%)	1 (0%)	24	63
2	K	214/340 (63%)	154 (72%)	58 (27%)	2 (1%)	14	51
3	H	214/539 (40%)	182 (85%)	32 (15%)	0	100	100
3	L	214/539 (40%)	163 (76%)	50 (23%)	1 (0%)	24	63
All	All	1712/3894 (44%)	1310 (76%)	398 (23%)	4 (0%)	44	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	129	GLN
3	L	138	LEU
2	G	139	VAL
2	K	138	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	187/472 (40%)	187 (100%)	0	100	100
1	F	187/472 (40%)	187 (100%)	0	100	100
1	I	187/472 (40%)	187 (100%)	0	100	100
1	J	187/472 (40%)	187 (100%)	0	100	100
2	G	173/278 (62%)	173 (100%)	0	100	100
2	K	173/278 (62%)	173 (100%)	0	100	100
3	H	175/451 (39%)	175 (100%)	0	100	100
3	L	175/451 (39%)	175 (100%)	0	100	100
All	All	1444/3346 (43%)	1444 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	52	HIS
1	F	46	ASN
2	G	74	GLN
2	G	174	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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-60986. These allow visual inspection of the internal detail of the map and identification of artifacts.

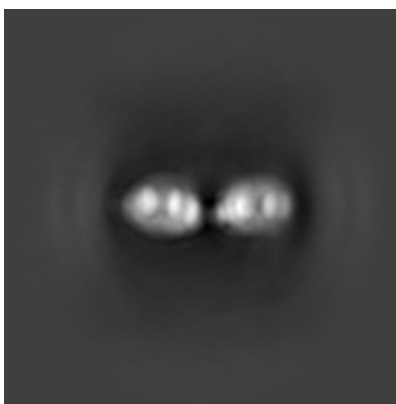
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

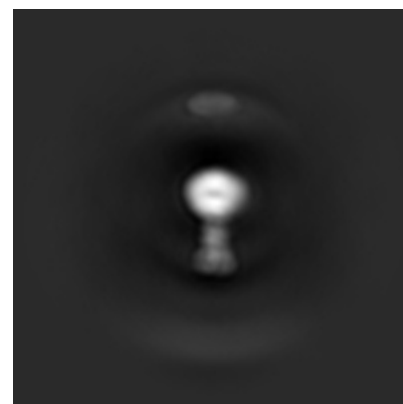
#### 6.1.1 Primary map



X

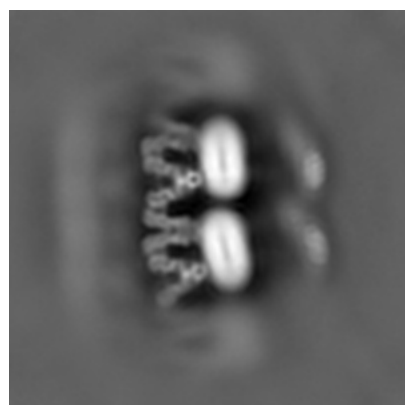


Y

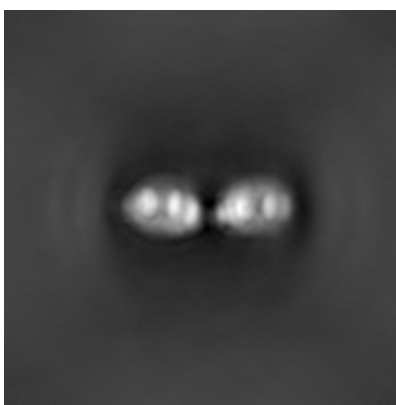


Z

#### 6.1.2 Raw map



X



Y

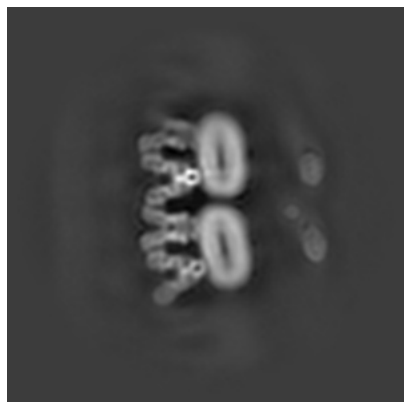


Z

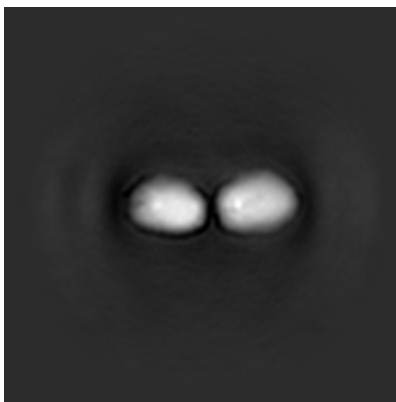
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

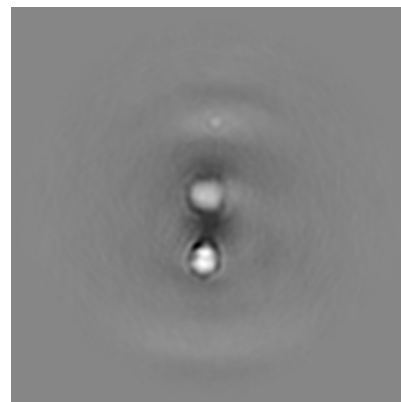
### 6.2.1 Primary map



X Index: 60

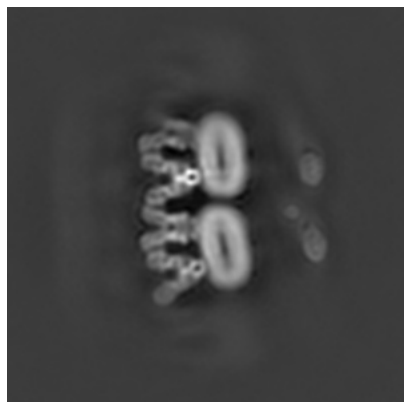


Y Index: 60

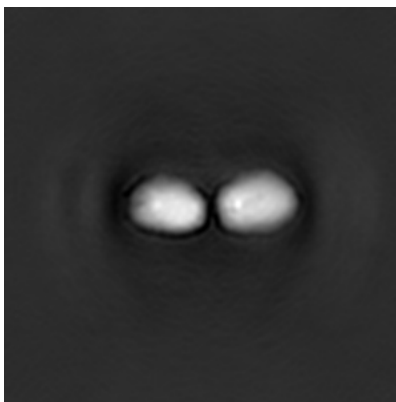


Z Index: 60

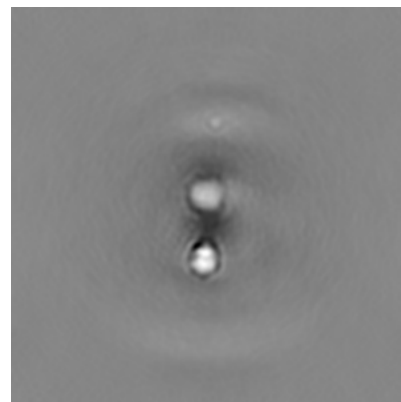
### 6.2.2 Raw map



X Index: 60



Y Index: 60

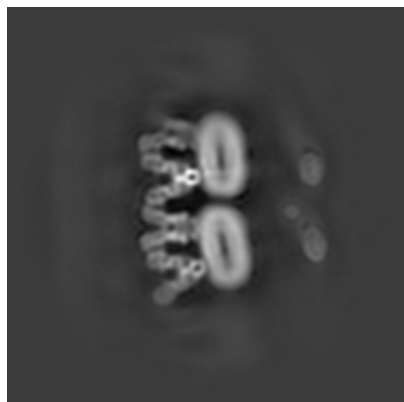


Z Index: 60

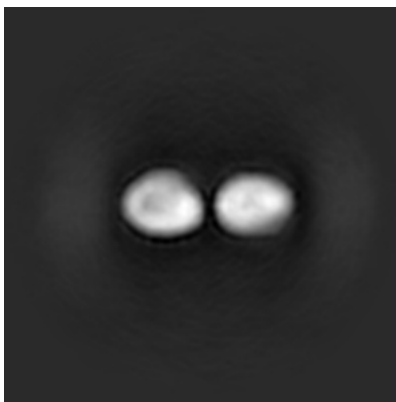
The images above show central slices of the map in three orthogonal directions.

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

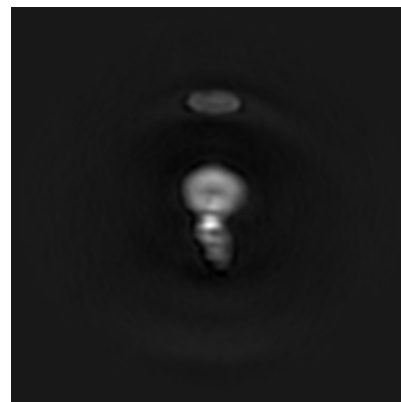
### 6.3.1 Primary map



X Index: 60

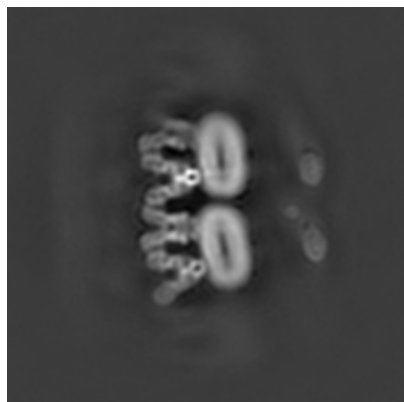


Y Index: 67

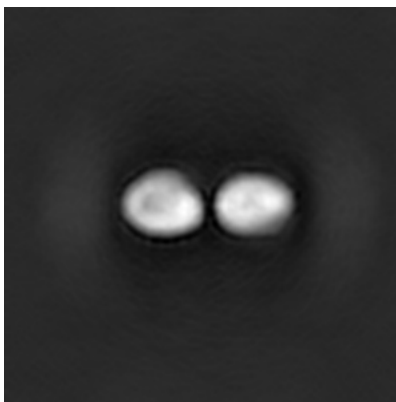


Z Index: 70

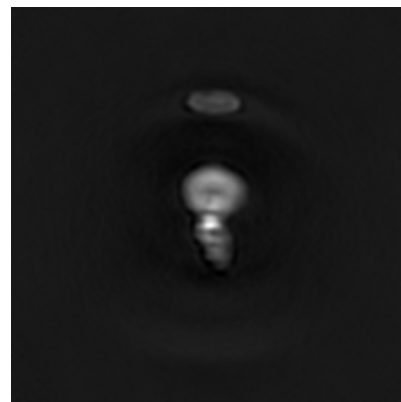
### 6.3.2 Raw map



X Index: 60



Y Index: 67



Z Index: 70

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

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

### 6.4.1 Primary map



X

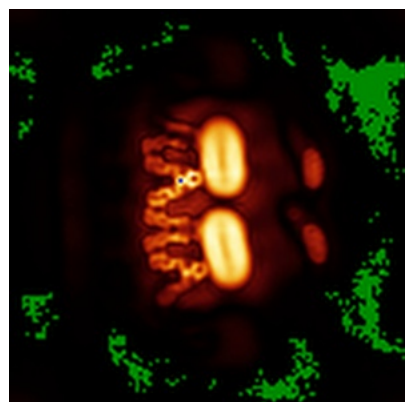


Y

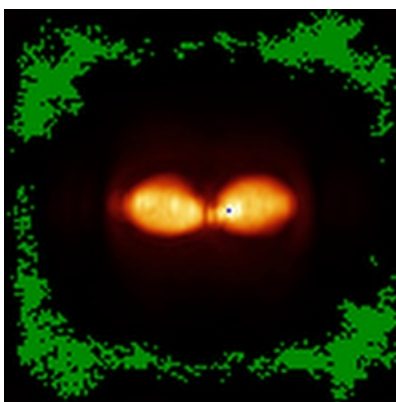


Z

### 6.4.2 Raw map



X



Y

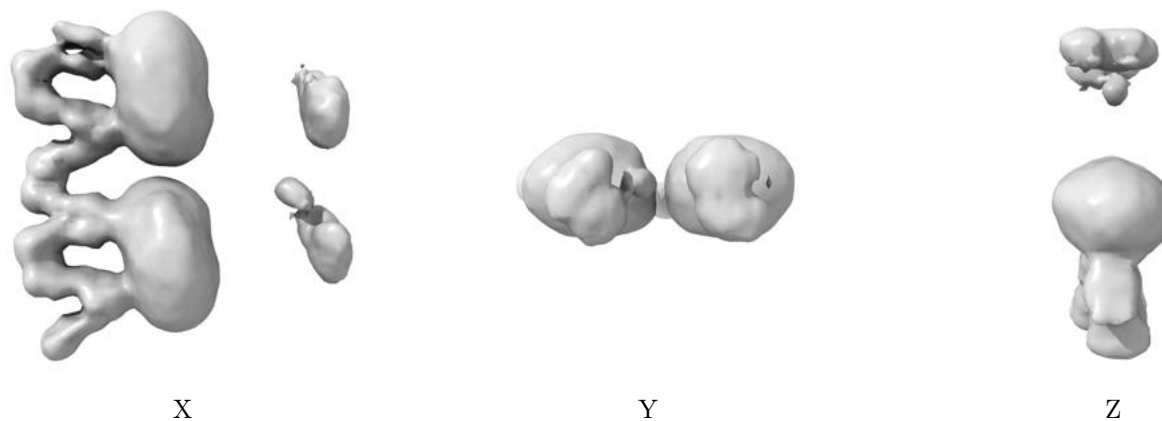


Z

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.

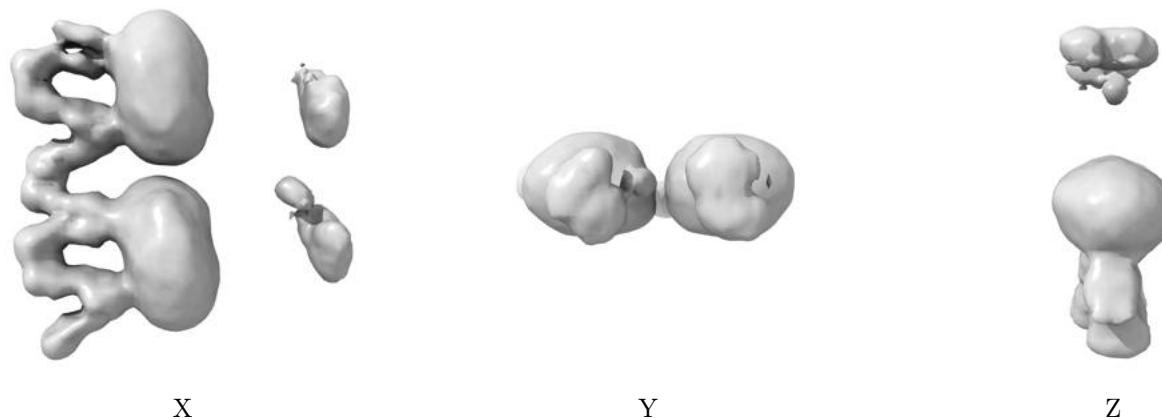
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

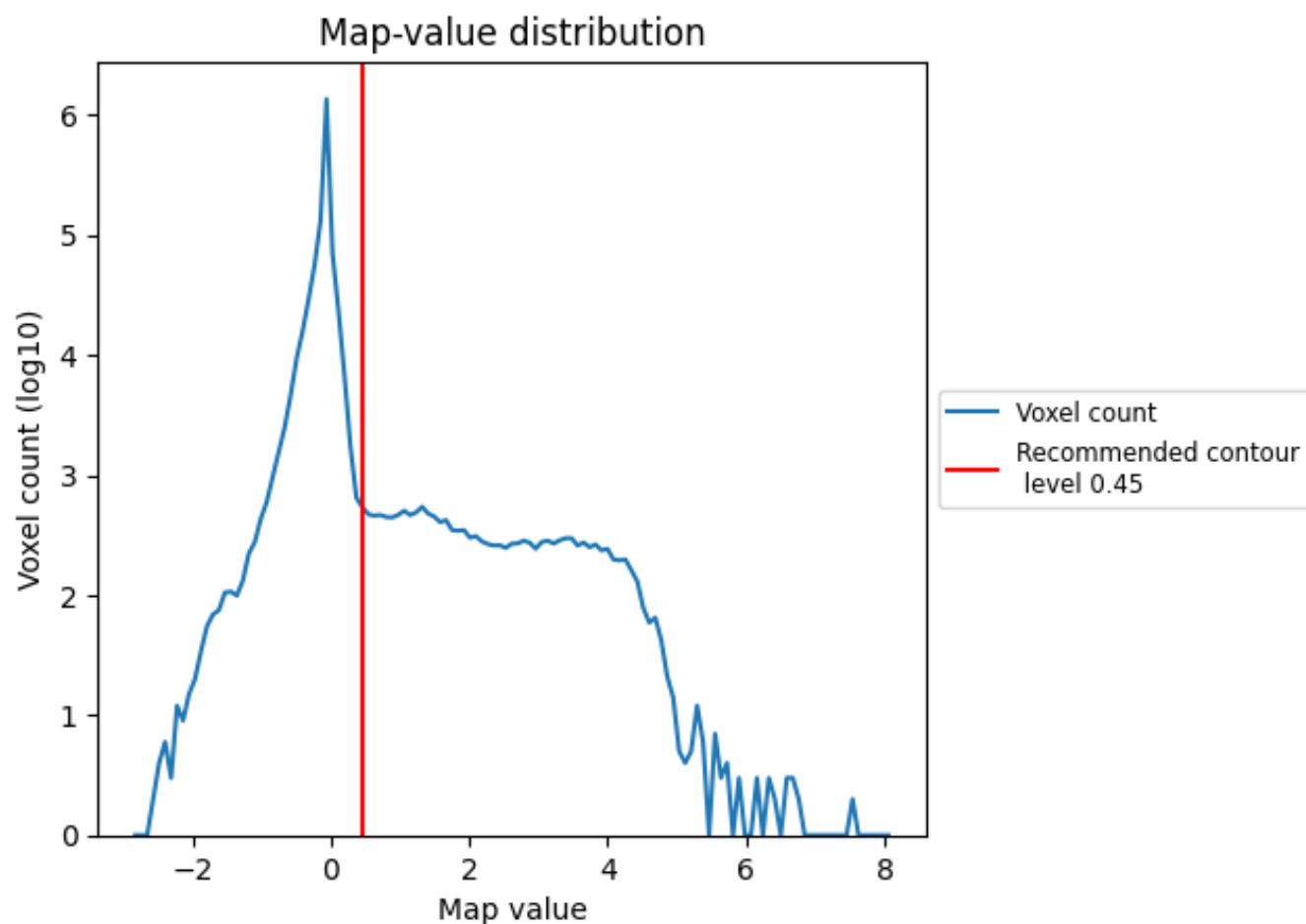
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

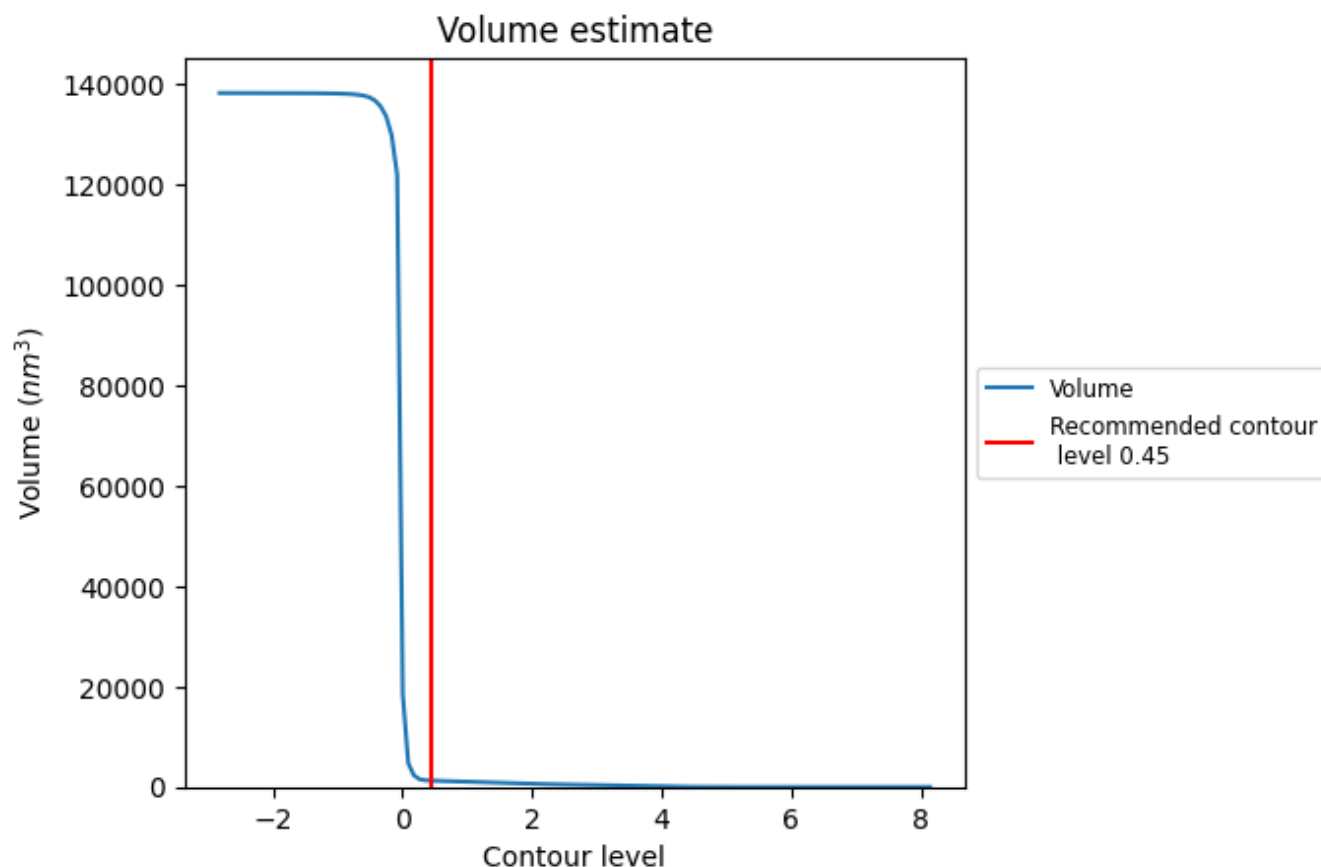
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

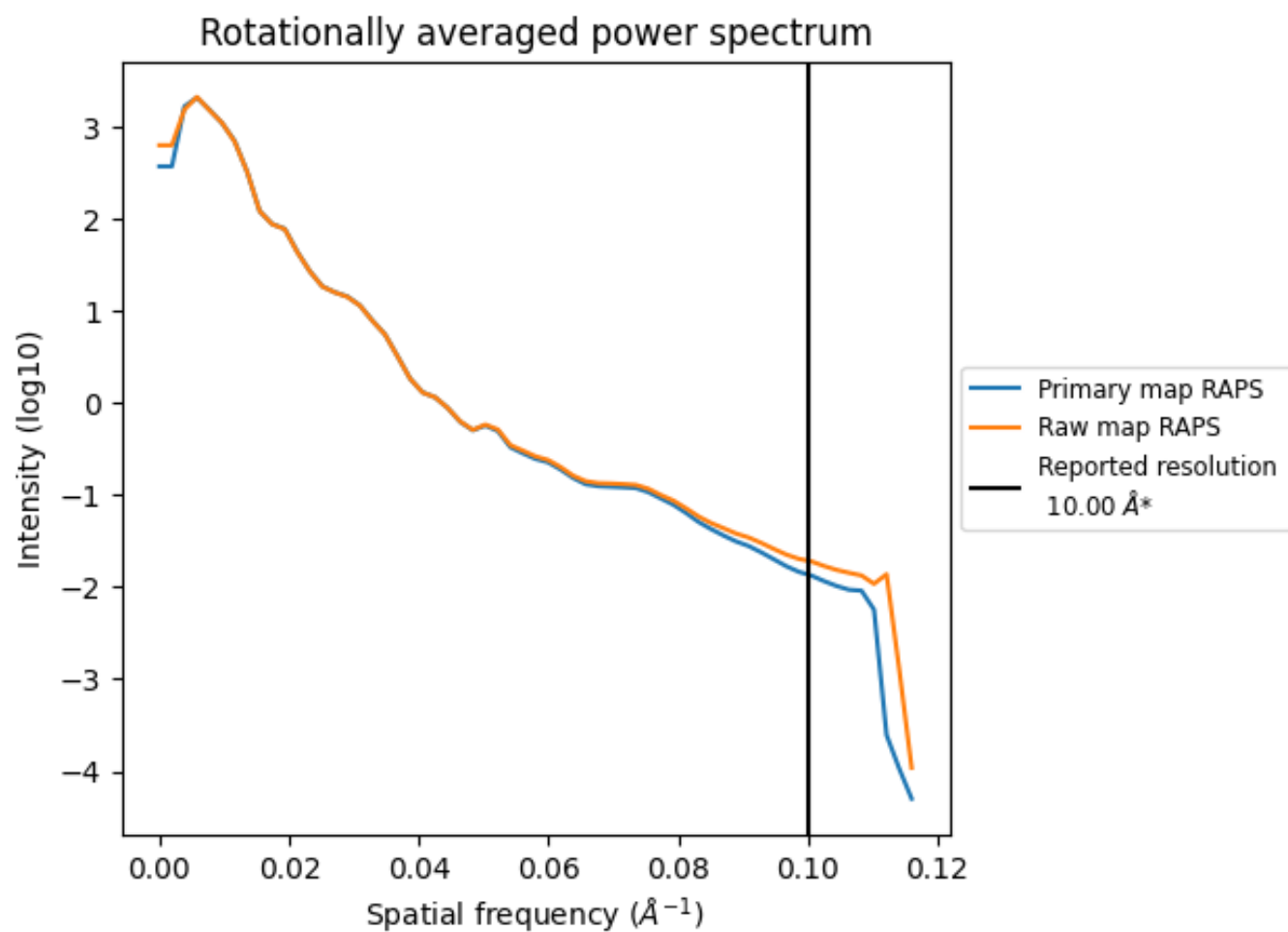
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1270  $\text{nm}^3$ ; this corresponds to an approximate mass of 1147 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 ⓘ



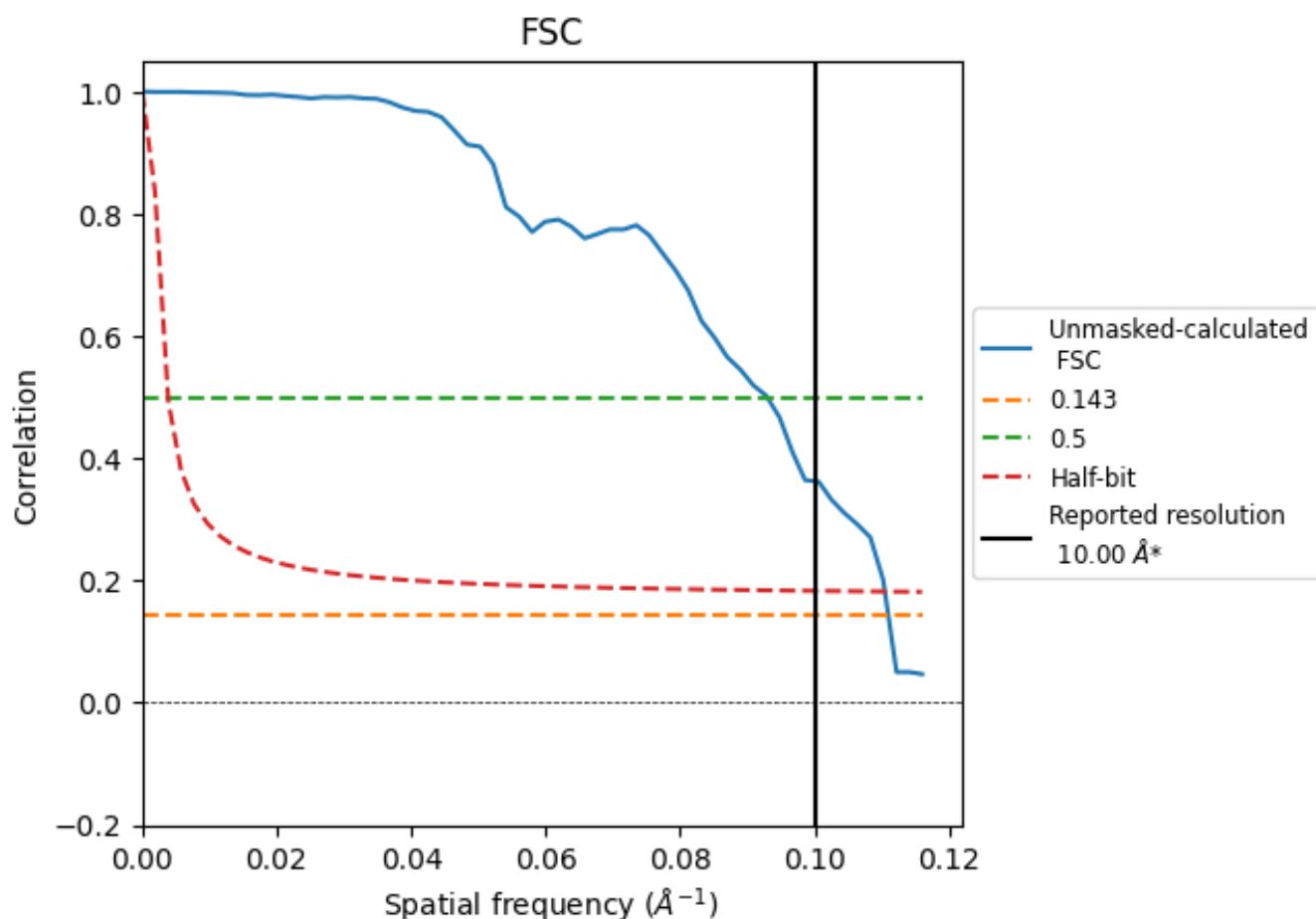
\*Reported resolution corresponds to spatial frequency of 0.100 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.100  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

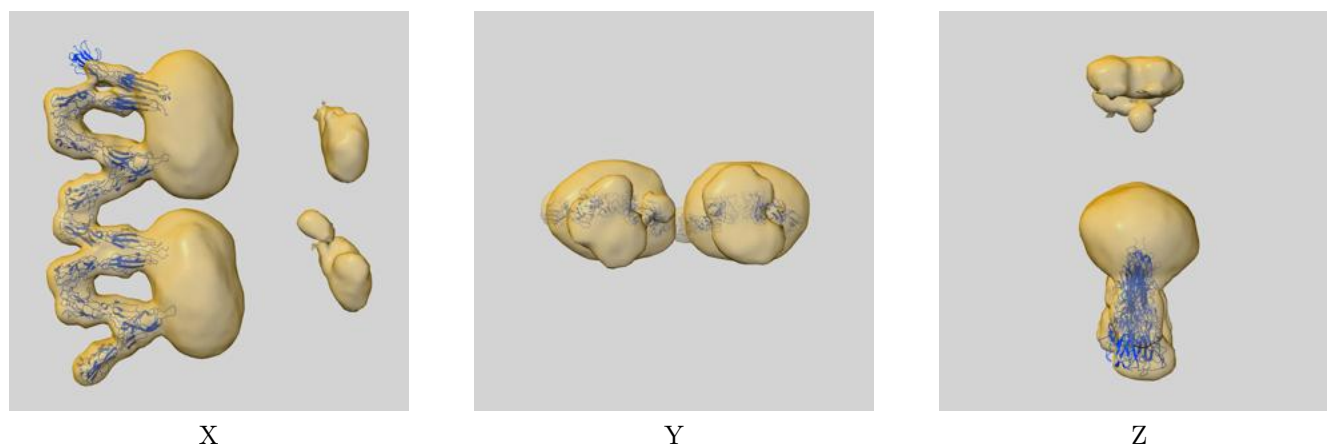
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.01	10.75	9.05

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

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

This section contains information regarding the fit between EMDB map EMD-60986 and PDB model 9IY6. Per-residue inclusion information can be found in section 3 on page 13.

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



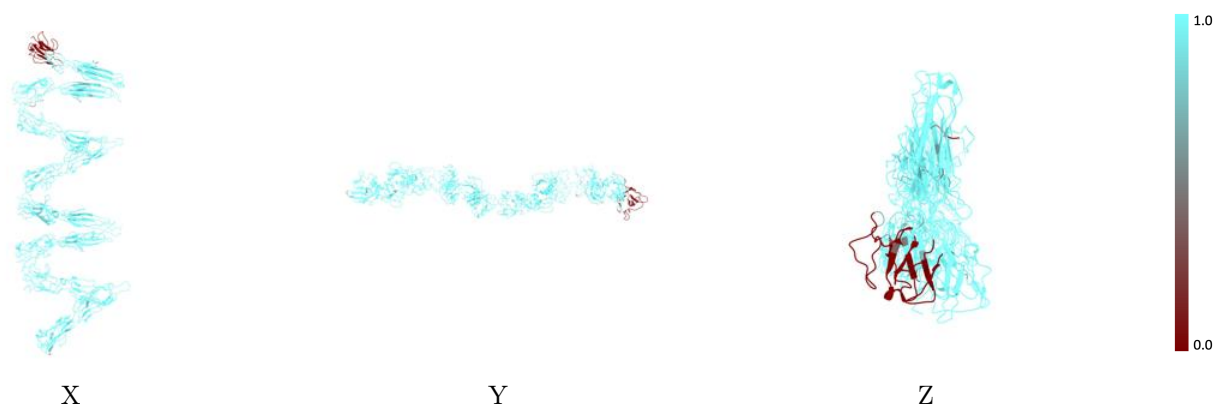
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



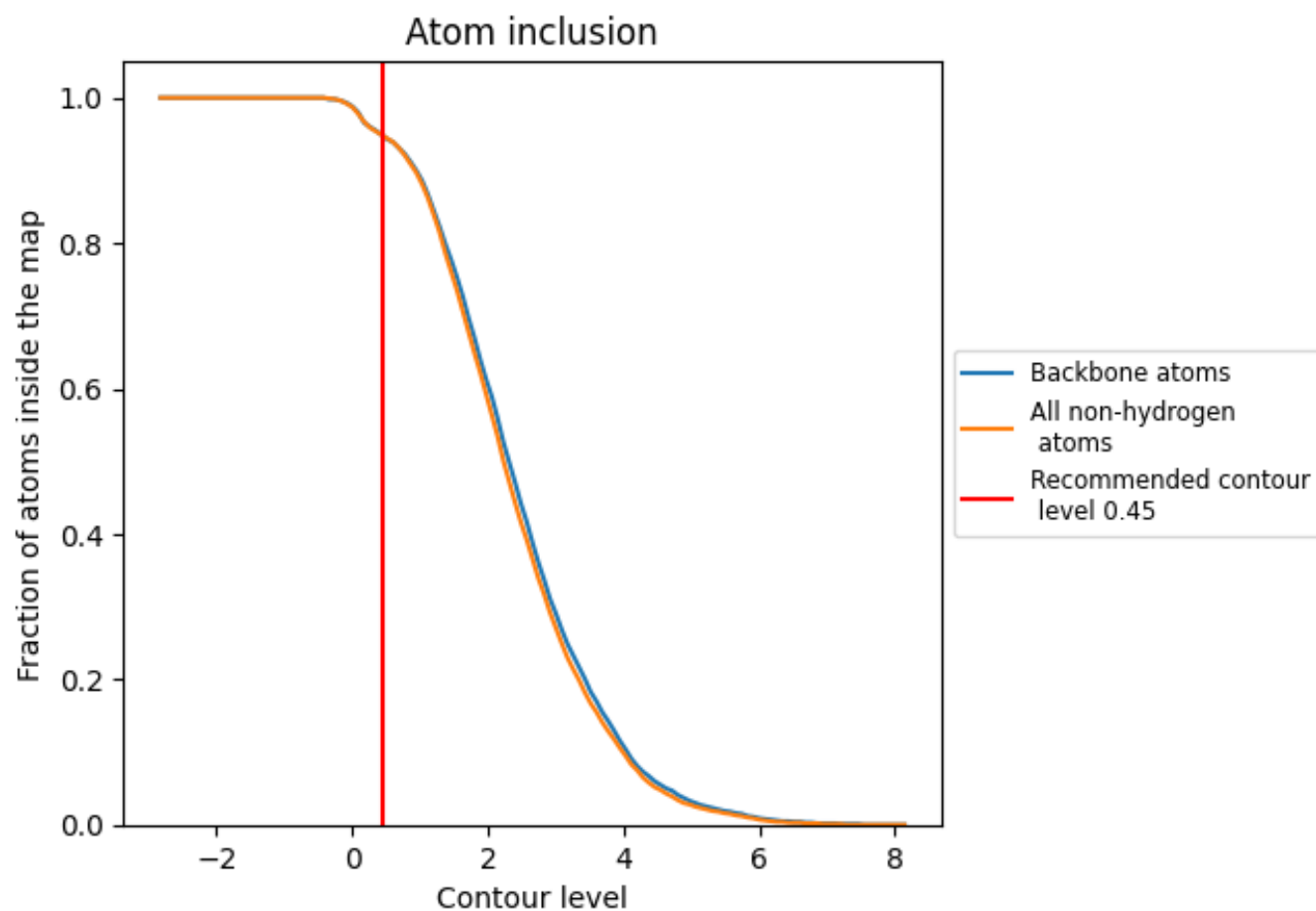
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9480	<div><div></div></div> 0.1070
E	<div><div></div></div> 1.0000	<div><div></div></div> 0.1240
F	<div><div></div></div> 1.0000	<div><div></div></div> 0.1170
G	<div><div></div></div> 0.9710	<div><div></div></div> 0.1040
H	<div><div></div></div> 0.6150	<div><div></div></div> 0.0850
I	<div><div></div></div> 0.9910	<div><div></div></div> 0.1060
J	<div><div></div></div> 1.0000	<div><div></div></div> 0.1120
K	<div><div></div></div> 1.0000	<div><div></div></div> 0.1040
L	<div><div></div></div> 1.0000	<div><div></div></div> 0.1020

1.0

0.0

<0.0