



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 08:47 PM UTC

PDB ID : 8BFN / pdb_00008bfm
EMDB ID : EMD-16020
Title : E. coli Wadjet JetABC dimer of dimers
Authors : Roisne-Hamelin, F.; Beckert, B.; Myasnikov, A.; Li, Y.; Gruber, S.
Deposited on : 2022-10-26
Resolution : 3.52 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

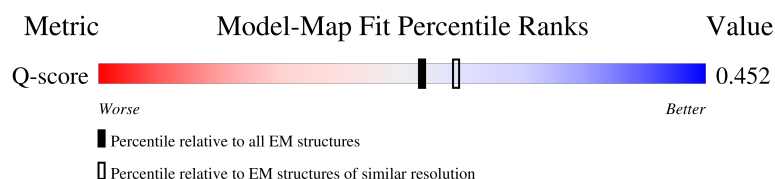
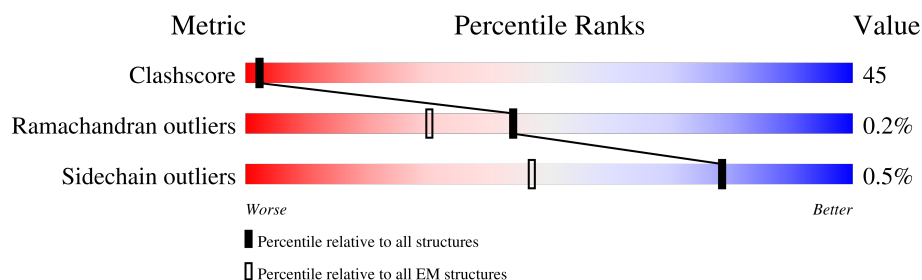
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.52 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	13017 (3.02 - 4.02)

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

Mol	Chain	Length	Quality of chain
1	A	1096	 5% 18% 27% 27% 46%
1	B	1096	 5% 18% 36% 46%
1	F	1096	 5% 18% 27% 27% 46%
1	G	1096	 5% 18% 36% 46%

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Mol	Chain	Length	Quality of chain
2	C	250	36%42%22%
2	D	250	38%39%22%
2	H	250	36%42%22%
2	I	250	37%41%22%
3	E	554	36%54%10%
3	J	554	38%52%10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33448 atoms, of which 48 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 JetC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		
1	B	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		
1	F	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		
1	G	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	GLN	conflict	UNP A0A4T5T6V2
A	298	SER	ASN	conflict	UNP A0A4T5T6V2
A	386	SER	ILE	conflict	UNP A0A4T5T6V2
A	398	GLU	ALA	conflict	UNP A0A4T5T6V2
A	400	ARG	LEU	conflict	UNP A0A4T5T6V2
A	576	HIS	ARG	conflict	UNP A0A4T5T6V2
A	625	ALA	THR	conflict	UNP A0A4T5T6V2
A	705	ILE	VAL	conflict	UNP A0A4T5T6V2
A	729	LEU	SER	conflict	UNP A0A4T5T6V2
A	823	PRO	THR	conflict	UNP A0A4T5T6V2
A	889	ASP	TYR	conflict	UNP A0A4T5T6V2
A	933	VAL	ILE	conflict	UNP A0A4T5T6V2
A	1096	GLY	-	insertion	UNP A0A4T5T6V2
B	283	LEU	GLN	conflict	UNP A0A4T5T6V2
B	298	SER	ASN	conflict	UNP A0A4T5T6V2
B	386	SER	ILE	conflict	UNP A0A4T5T6V2
B	398	GLU	ALA	conflict	UNP A0A4T5T6V2
B	400	ARG	LEU	conflict	UNP A0A4T5T6V2
B	576	HIS	ARG	conflict	UNP A0A4T5T6V2
B	625	ALA	THR	conflict	UNP A0A4T5T6V2
B	705	ILE	VAL	conflict	UNP A0A4T5T6V2
B	729	LEU	SER	conflict	UNP A0A4T5T6V2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	823	PRO	THR	conflict	UNP A0A4T5T6V2
B	889	ASP	TYR	conflict	UNP A0A4T5T6V2
B	933	VAL	ILE	conflict	UNP A0A4T5T6V2
B	1096	GLY	-	insertion	UNP A0A4T5T6V2
F	283	LEU	GLN	conflict	UNP A0A4T5T6V2
F	298	SER	ASN	conflict	UNP A0A4T5T6V2
F	386	SER	ILE	conflict	UNP A0A4T5T6V2
F	398	GLU	ALA	conflict	UNP A0A4T5T6V2
F	400	ARG	LEU	conflict	UNP A0A4T5T6V2
F	576	HIS	ARG	conflict	UNP A0A4T5T6V2
F	625	ALA	THR	conflict	UNP A0A4T5T6V2
F	705	ILE	VAL	conflict	UNP A0A4T5T6V2
F	729	LEU	SER	conflict	UNP A0A4T5T6V2
F	823	PRO	THR	conflict	UNP A0A4T5T6V2
F	889	ASP	TYR	conflict	UNP A0A4T5T6V2
F	933	VAL	ILE	conflict	UNP A0A4T5T6V2
F	1096	GLY	-	insertion	UNP A0A4T5T6V2
G	283	LEU	GLN	conflict	UNP A0A4T5T6V2
G	298	SER	ASN	conflict	UNP A0A4T5T6V2
G	386	SER	ILE	conflict	UNP A0A4T5T6V2
G	398	GLU	ALA	conflict	UNP A0A4T5T6V2
G	400	ARG	LEU	conflict	UNP A0A4T5T6V2
G	576	HIS	ARG	conflict	UNP A0A4T5T6V2
G	625	ALA	THR	conflict	UNP A0A4T5T6V2
G	705	ILE	VAL	conflict	UNP A0A4T5T6V2
G	729	LEU	SER	conflict	UNP A0A4T5T6V2
G	823	PRO	THR	conflict	UNP A0A4T5T6V2
G	889	ASP	TYR	conflict	UNP A0A4T5T6V2
G	933	VAL	ILE	conflict	UNP A0A4T5T6V2
G	1096	GLY	-	insertion	UNP A0A4T5T6V2

- Molecule 2 is a protein called JetB.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	195	Total	C	N	O	0	0
			1566	991	280	295		
2	D	195	Total	C	N	O	0	0
			1566	991	280	295		
2	H	195	Total	C	N	O	0	0
			1566	991	280	295		
2	I	195	Total	C	N	O	0	0
			1566	991	280	295		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	THR	conflict	UNP A0A4C9B499
C	7	LYS	ARG	conflict	UNP A0A4C9B499
C	35	ASP	GLU	conflict	UNP A0A4C9B499
C	46	GLN	LYS	conflict	UNP A0A4C9B499
C	240	PRO	ARG	conflict	UNP A0A4C9B499
C	250	GLY	-	insertion	UNP A0A4C9B499
D	2	ALA	THR	conflict	UNP A0A4C9B499
D	7	LYS	ARG	conflict	UNP A0A4C9B499
D	35	ASP	GLU	conflict	UNP A0A4C9B499
D	46	GLN	LYS	conflict	UNP A0A4C9B499
D	240	PRO	ARG	conflict	UNP A0A4C9B499
D	250	GLY	-	insertion	UNP A0A4C9B499
H	2	ALA	THR	conflict	UNP A0A4C9B499
H	7	LYS	ARG	conflict	UNP A0A4C9B499
H	35	ASP	GLU	conflict	UNP A0A4C9B499
H	46	GLN	LYS	conflict	UNP A0A4C9B499
H	240	PRO	ARG	conflict	UNP A0A4C9B499
H	250	GLY	-	insertion	UNP A0A4C9B499
I	2	ALA	THR	conflict	UNP A0A4C9B499
I	7	LYS	ARG	conflict	UNP A0A4C9B499
I	35	ASP	GLU	conflict	UNP A0A4C9B499
I	46	GLN	LYS	conflict	UNP A0A4C9B499
I	240	PRO	ARG	conflict	UNP A0A4C9B499
I	250	GLY	-	insertion	UNP A0A4C9B499

- Molecule 3 is a protein called JetA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	498	Total	C	N	O	S	0	0
			4044	2512	752	772	8		
3	J	498	Total	C	N	O	S	0	0
			4044	2512	752	772	8		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-54	MET	-	initiating methionine	UNP A0A4V3QHV5
E	-53	ALA	-	expression tag	UNP A0A4V3QHV5
E	-52	HIS	-	expression tag	UNP A0A4V3QHV5
E	-51	HIS	-	expression tag	UNP A0A4V3QHV5
E	-50	HIS	-	expression tag	UNP A0A4V3QHV5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-49	HIS	-	expression tag	UNP A0A4V3QHV5
E	-48	HIS	-	expression tag	UNP A0A4V3QHV5
E	-47	HIS	-	expression tag	UNP A0A4V3QHV5
E	-46	HIS	-	expression tag	UNP A0A4V3QHV5
E	-45	HIS	-	expression tag	UNP A0A4V3QHV5
E	-44	HIS	-	expression tag	UNP A0A4V3QHV5
E	-43	HIS	-	expression tag	UNP A0A4V3QHV5
E	-42	GLY	-	expression tag	UNP A0A4V3QHV5
E	-41	GLY	-	expression tag	UNP A0A4V3QHV5
E	-40	SER	-	expression tag	UNP A0A4V3QHV5
E	-39	SER	-	expression tag	UNP A0A4V3QHV5
E	-38	ALA	-	expression tag	UNP A0A4V3QHV5
E	-37	TRP	-	expression tag	UNP A0A4V3QHV5
E	-36	SER	-	expression tag	UNP A0A4V3QHV5
E	-35	HIS	-	expression tag	UNP A0A4V3QHV5
E	-34	PRO	-	expression tag	UNP A0A4V3QHV5
E	-33	GLN	-	expression tag	UNP A0A4V3QHV5
E	-32	PHE	-	expression tag	UNP A0A4V3QHV5
E	-31	GLU	-	expression tag	UNP A0A4V3QHV5
E	-30	LYS	-	expression tag	UNP A0A4V3QHV5
E	-29	GLY	-	expression tag	UNP A0A4V3QHV5
E	-28	GLY	-	expression tag	UNP A0A4V3QHV5
E	-27	GLY	-	expression tag	UNP A0A4V3QHV5
E	-26	SER	-	expression tag	UNP A0A4V3QHV5
E	-25	GLY	-	expression tag	UNP A0A4V3QHV5
E	-24	GLY	-	expression tag	UNP A0A4V3QHV5
E	-23	GLY	-	expression tag	UNP A0A4V3QHV5
E	-22	SER	-	expression tag	UNP A0A4V3QHV5
E	-21	GLY	-	expression tag	UNP A0A4V3QHV5
E	-20	GLY	-	expression tag	UNP A0A4V3QHV5
E	-19	GLY	-	expression tag	UNP A0A4V3QHV5
E	-18	SER	-	expression tag	UNP A0A4V3QHV5
E	-17	TRP	-	expression tag	UNP A0A4V3QHV5
E	-16	SER	-	expression tag	UNP A0A4V3QHV5
E	-15	HIS	-	expression tag	UNP A0A4V3QHV5
E	-14	PRO	-	expression tag	UNP A0A4V3QHV5
E	-13	GLN	-	expression tag	UNP A0A4V3QHV5
E	-12	PHE	-	expression tag	UNP A0A4V3QHV5
E	-11	GLU	-	expression tag	UNP A0A4V3QHV5
E	-10	LYS	-	expression tag	UNP A0A4V3QHV5
E	-9	LEU	-	expression tag	UNP A0A4V3QHV5
E	-8	GLU	-	expression tag	UNP A0A4V3QHV5

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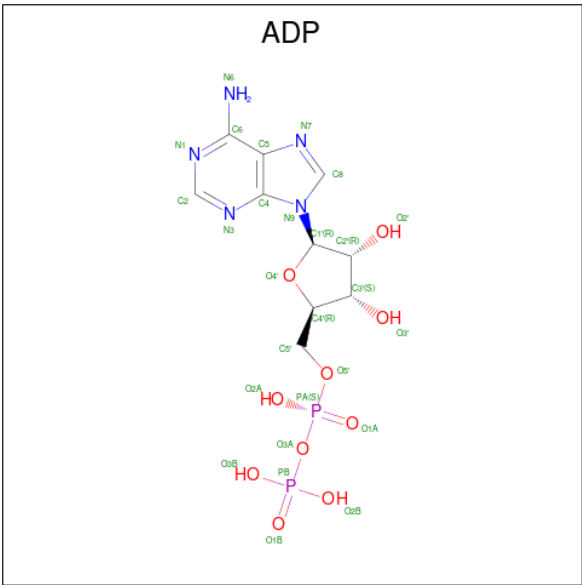
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	VAL	-	expression tag	UNP A0A4V3QHV5
E	-6	LEU	-	expression tag	UNP A0A4V3QHV5
E	-5	PHE	-	expression tag	UNP A0A4V3QHV5
E	-4	GLN	-	expression tag	UNP A0A4V3QHV5
E	-3	GLY	-	expression tag	UNP A0A4V3QHV5
E	-2	PRO	-	expression tag	UNP A0A4V3QHV5
E	-1	ALA	-	expression tag	UNP A0A4V3QHV5
E	0	ALA	-	expression tag	UNP A0A4V3QHV5
E	187	ASP	GLU	conflict	UNP A0A4V3QHV5
E	435	GLU	ALA	conflict	UNP A0A4V3QHV5
E	499	GLY	-	insertion	UNP A0A4V3QHV5
J	-54	MET	-	initiating methionine	UNP A0A4V3QHV5
J	-53	ALA	-	expression tag	UNP A0A4V3QHV5
J	-52	HIS	-	expression tag	UNP A0A4V3QHV5
J	-51	HIS	-	expression tag	UNP A0A4V3QHV5
J	-50	HIS	-	expression tag	UNP A0A4V3QHV5
J	-49	HIS	-	expression tag	UNP A0A4V3QHV5
J	-48	HIS	-	expression tag	UNP A0A4V3QHV5
J	-47	HIS	-	expression tag	UNP A0A4V3QHV5
J	-46	HIS	-	expression tag	UNP A0A4V3QHV5
J	-45	HIS	-	expression tag	UNP A0A4V3QHV5
J	-44	HIS	-	expression tag	UNP A0A4V3QHV5
J	-43	HIS	-	expression tag	UNP A0A4V3QHV5
J	-42	GLY	-	expression tag	UNP A0A4V3QHV5
J	-41	GLY	-	expression tag	UNP A0A4V3QHV5
J	-40	SER	-	expression tag	UNP A0A4V3QHV5
J	-39	SER	-	expression tag	UNP A0A4V3QHV5
J	-38	ALA	-	expression tag	UNP A0A4V3QHV5
J	-37	TRP	-	expression tag	UNP A0A4V3QHV5
J	-36	SER	-	expression tag	UNP A0A4V3QHV5
J	-35	HIS	-	expression tag	UNP A0A4V3QHV5
J	-34	PRO	-	expression tag	UNP A0A4V3QHV5
J	-33	GLN	-	expression tag	UNP A0A4V3QHV5
J	-32	PHE	-	expression tag	UNP A0A4V3QHV5
J	-31	GLU	-	expression tag	UNP A0A4V3QHV5
J	-30	LYS	-	expression tag	UNP A0A4V3QHV5
J	-29	GLY	-	expression tag	UNP A0A4V3QHV5
J	-28	GLY	-	expression tag	UNP A0A4V3QHV5
J	-27	GLY	-	expression tag	UNP A0A4V3QHV5
J	-26	SER	-	expression tag	UNP A0A4V3QHV5
J	-25	GLY	-	expression tag	UNP A0A4V3QHV5
J	-24	GLY	-	expression tag	UNP A0A4V3QHV5

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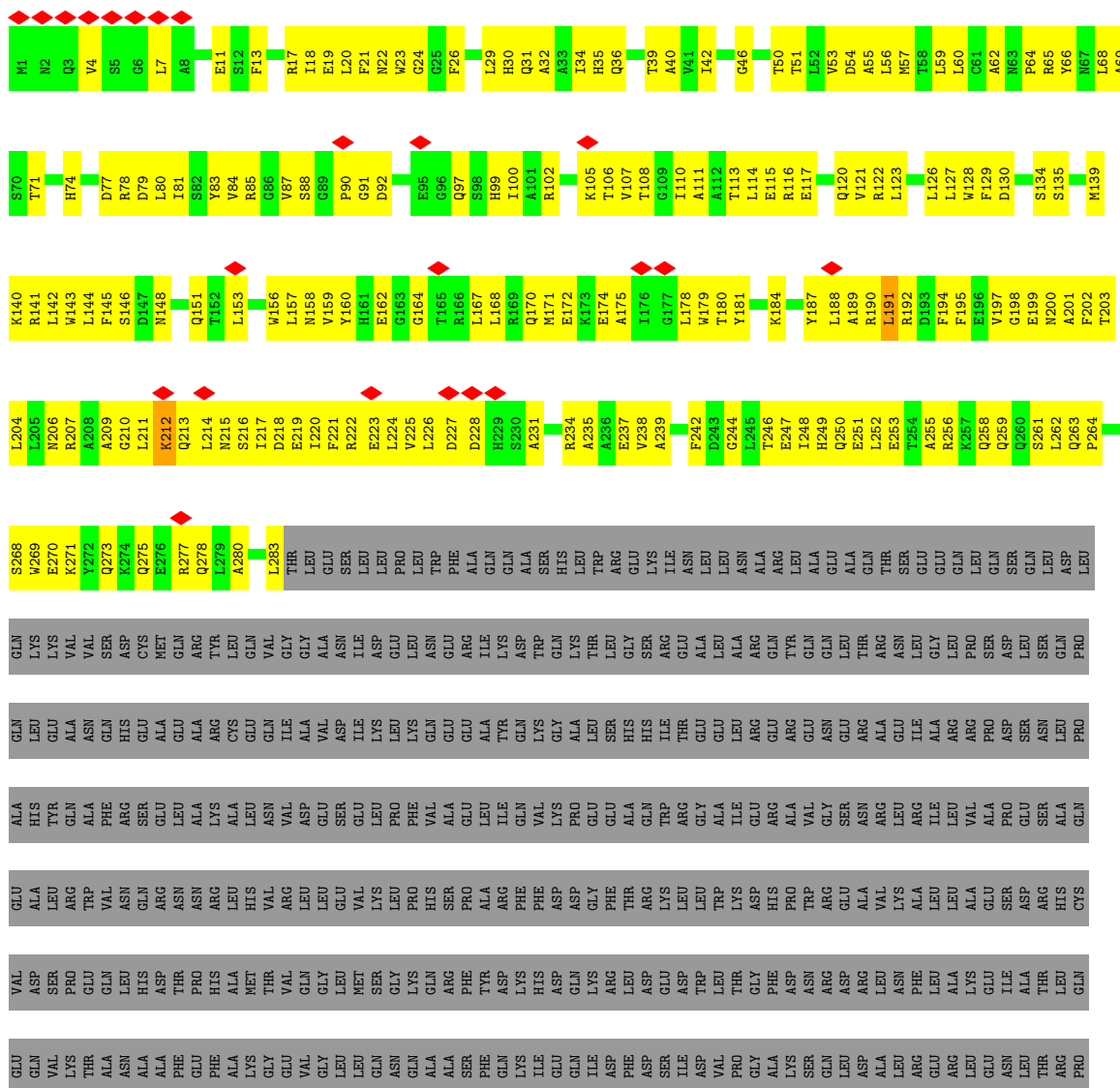
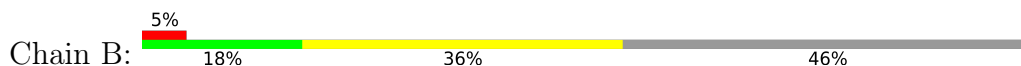
Chain	Residue	Modelled	Actual	Comment	Reference
J	-23	GLY	-	expression tag	UNP A0A4V3QHV5
J	-22	SER	-	expression tag	UNP A0A4V3QHV5
J	-21	GLY	-	expression tag	UNP A0A4V3QHV5
J	-20	GLY	-	expression tag	UNP A0A4V3QHV5
J	-19	GLY	-	expression tag	UNP A0A4V3QHV5
J	-18	SER	-	expression tag	UNP A0A4V3QHV5
J	-17	TRP	-	expression tag	UNP A0A4V3QHV5
J	-16	SER	-	expression tag	UNP A0A4V3QHV5
J	-15	HIS	-	expression tag	UNP A0A4V3QHV5
J	-14	PRO	-	expression tag	UNP A0A4V3QHV5
J	-13	GLN	-	expression tag	UNP A0A4V3QHV5
J	-12	PHE	-	expression tag	UNP A0A4V3QHV5
J	-11	GLU	-	expression tag	UNP A0A4V3QHV5
J	-10	LYS	-	expression tag	UNP A0A4V3QHV5
J	-9	LEU	-	expression tag	UNP A0A4V3QHV5
J	-8	GLU	-	expression tag	UNP A0A4V3QHV5
J	-7	VAL	-	expression tag	UNP A0A4V3QHV5
J	-6	LEU	-	expression tag	UNP A0A4V3QHV5
J	-5	PHE	-	expression tag	UNP A0A4V3QHV5
J	-4	GLN	-	expression tag	UNP A0A4V3QHV5
J	-3	GLY	-	expression tag	UNP A0A4V3QHV5
J	-2	PRO	-	expression tag	UNP A0A4V3QHV5
J	-1	ALA	-	expression tag	UNP A0A4V3QHV5
J	0	ALA	-	expression tag	UNP A0A4V3QHV5
J	187	ASP	GLU	conflict	UNP A0A4V3QHV5
J	435	GLU	ALA	conflict	UNP A0A4V3QHV5
J	499	GLY	-	insertion	UNP A0A4V3QHV5

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

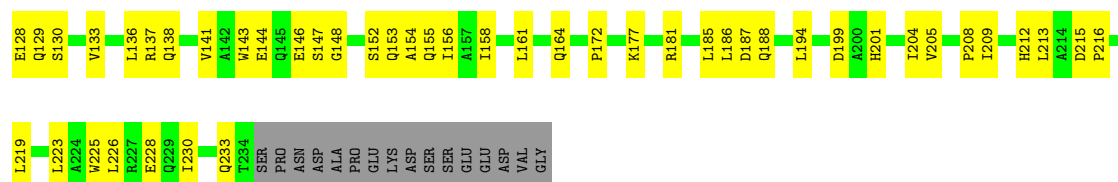


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	G	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 1: JetC



W	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO	BP	BQ	BR	BS	BT	BV	BW	BX	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR	CS	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG	DH	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DV	DW	DX	DY	DZ	EA	EB	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL	EM	EN	EO	EP	EQ	ER	ES	ET	EU	EV	EW	EX	EY	EZ	FA	FB	FC	FD	FE	FF	FG	FH	FI	FJ	FK	FL	FM	FN	FO	FP	FQ	FR	FS	FT	FV	FW	FX	FY	FZ	GA	GB	GC	GD	GE	GF	GG	GH	GI	GJ	GK	GL	GM	GN	GO	GP	GQ	GR	GS	GT	GV	GW	GX	GY	GZ	HA	HB	HC	HD	HE	HF	HG	HH	HI	HJ	HK	HL	HM	HN	HO	HP	HQ	HR	HS	HT	HV	HW	HX	HY	HZ	IA	IB	IC	ID	IE	IF	IG	IH	II	IJ	IK	IL	IM	IN	IO	IP	IQ	IR	IS	IT	IV	IW	IX	IY	IZ	JA	JB	JC	JD	JE	JF	JG	JH	JI	IJ	JK	JL	JM	JN	JO	JP	JQ	JR	JS	JT	JV	JW	JX	JY	JZ	KA	KB	KC	KD	KE	KF	KG	KH	KI	KJ	KK	KL	KM	KN	KO	KP	KQ	KR	KS	KT	KV	KW	KX	KY	KZ	LA	LB	LC	LD	LE	LF	LG	LH	LI	LJ	LK	LM	LN	LO	LP	LQ	LR	LS	LT	LV	LW	LX	LY	LZ	MA	MB	MC	MD	ME	MF	MG	MH	MI	MJ	MK	ML	MM	MN	MO	MP	MQ	MR	MS	MT	MV	MW	MX	MY	MZ	NA	NB	NC	ND	NE	NF	NG	NH	NI	NJ	NK	NL	NM	NN	NO	NP	NQ	NR	NS	NT	NV	NW	NX	NY	NZ	OA	OB	OC	OD	OE	OF	OG	OH	OI	OJ	OK	OL	OM	ON	OO	OP	OQ	OR	OS	OT	OV	OW	OX	OY	OZ	PA	PB	PC	PD	PE	PF	PG	PH	PI	PJ	PK	PL	PM	PN	PO	PP	PQ	PR	PS	PT	PV	PW	PX	PY	PZ	QA	QB	QC	QD	QE	QF	QG	QH	QI	QJ	QK	QL	QM	QN	QO	QP	QR	QS	QT	QV	QW	QX	QY	QZ	RA	RB	RC	RD	RE	RF	RG	RH	RI	RJ	RK	RL	RM	RN	RO	RP	RQ	RR	RS	RT	RV	RW	RX	RY	RZ	SA	SB	SC	SD	SE	SF	SG	SH	SI	SJ	SK	SL	SM	SN	SO	SP	SQ	SR	SS	ST	SV	SW	SX	SY	SZ	TA	TB	TC	TD	TE	TF	TG	TH	TI	TJ	TK	TL	TM	TN	TO	TP	TQ	TR	TS	TV	TW	TX	TY	TZ	UA	UB	UC	UD	UE	UF	UG	UH	UI	UJ	UK	UL	UM	UN	UO	UP	UQ	UR	US	UT	UV	UW	UX	UY	UZ	VA	VB	VC	VD	VE	VF	VG	VH	VI	VJ	VK	VL	VM	VN	VO	VP	VQ	VR	VS	VT	VV	VW	VX	VY	VZ	WA	WB	WC	WD	WE	WF	WG	WH	WI	WJ	WK	WL	WM	WN	WO	WP	WQ	WR	WS	WT	WV	WW	WX	WY	WZ	XA	XB	XC	XD	XE	XF	XG	XH	XI	XJ	XK	XL	XM	XN	XO	XP	XQ	XR	XS	XT	XV	XW	XX	XY	XZ	YA	YB	YC	YD	YE	YF	YG	YH	YI	YJ	YK	YL	YM	YN	YO	YP	YQ	YR	YS	YT	YV	YW	YX	YZ	ZA	ZB	ZC	ZD	ZE	ZF	ZG	ZH	ZI	ZJ	ZK	ZL	ZM	ZN	ZO	ZP	ZQ	ZR	ZS	ZT	ZV	ZW	ZX	ZY	ZZ
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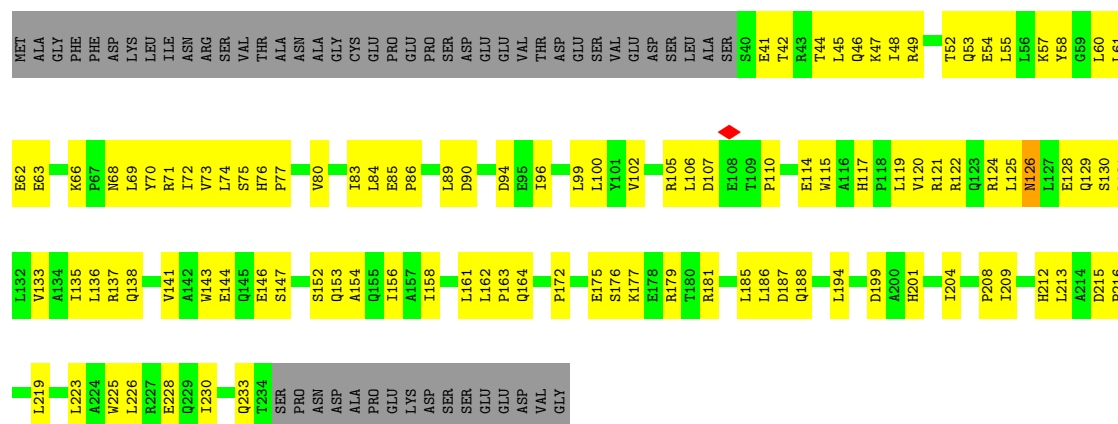
• Molecule 2: JetB

Chain D: 38% 39% 22%



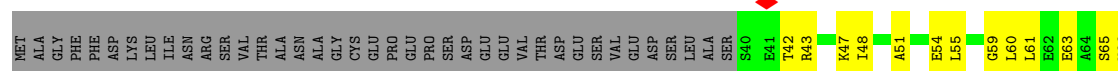
• Molecule 2: JetB

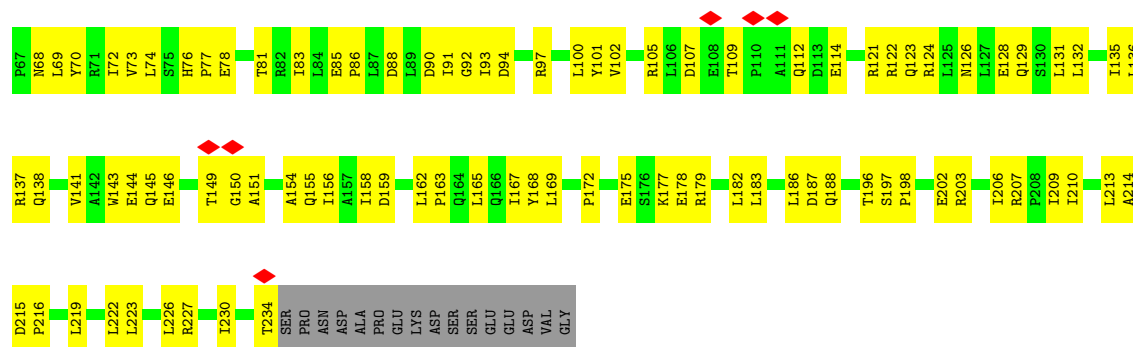
Chain H: 36% 42% 22%



• Molecule 2: JetB

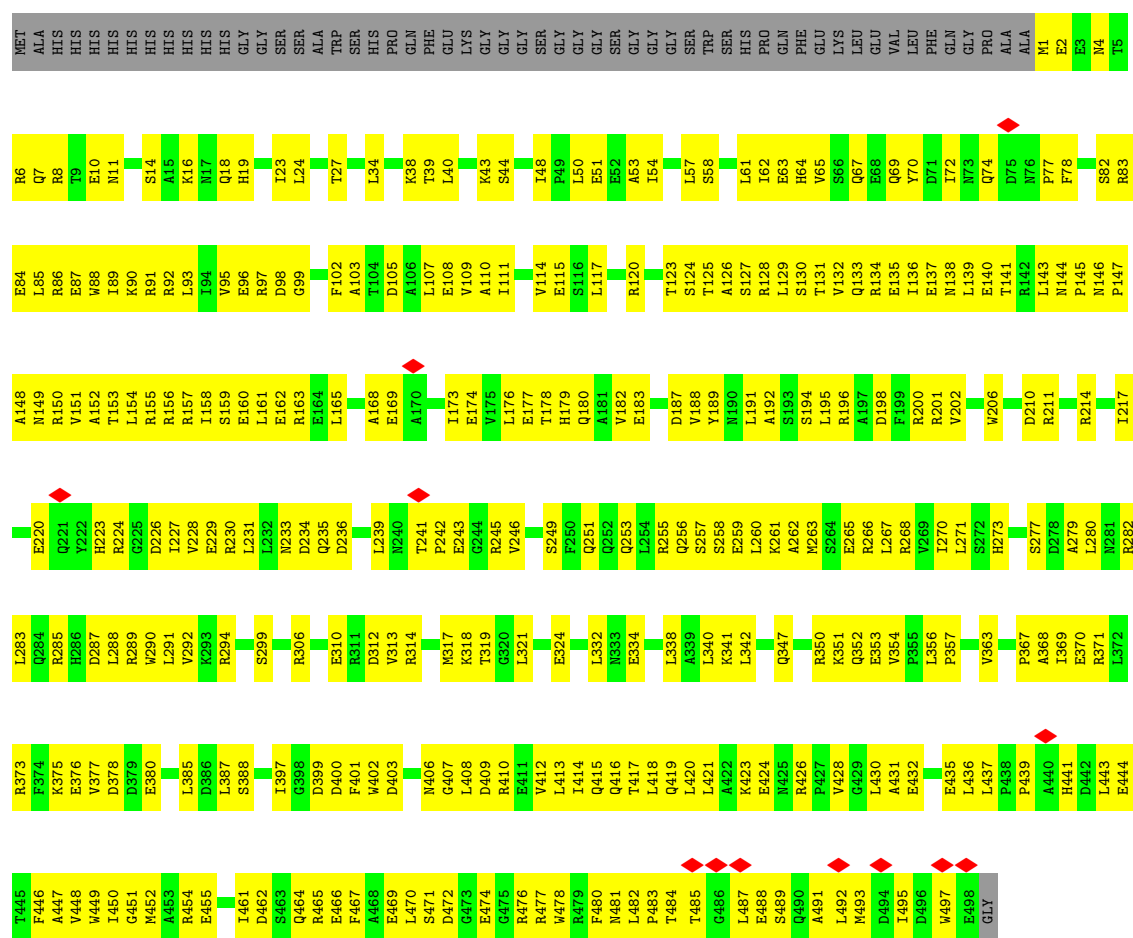
Chain I: 37% 41% 22%





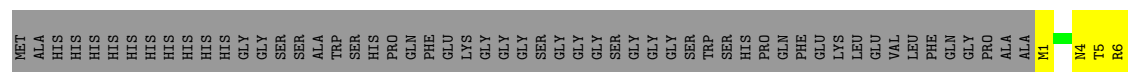
• Molecule 3: JetA

Chain E: 36% 54% 10%



• Molecule 3: JetA

Chain J: 38% 52% 10%



L385	E459	L295	E229	R155	Q7
D386	V460	V296	R230	R156	R8
L387	L387	S299	N233	R157	T9
S388	I461	Q300	D234	I158	E10
I397	D462	R306	Q235	S159	N11
Q464	S463	R306	D236	E160	S14
D400	Q464	E310	L239	L161	A15
F401	E466	R314	N240	E162	V95
W402	E466	V313	T241	R163	E96
F405	E469	R314	P242	E164	N17
N406	S471	L321	E243	L165	Q18
G407	D472	M317	G244	A168	H19
L408	G473	K318	R245	E169	I23
D409	E474	T319	V246	A170	L24
R410	G475	G320	F247	D105	T27
E411	R476	L321	D248	I173	L34
V412	R477	E324	S249	V175	E108
L413	W478	E324	F250	L176	V109
I414	R479	V328	Q251	E177	A110
Q415	F480	V328	R255	T178	I111
Q416	N481	L332	Q256	H179	V114
T417	L482	N333	Q256	Q180	E115
L418	P483	E334	S257	A181	S116
Q419	T484	L342	S258	V182	L117
L420	T485	L338	E259		L50
L421	G486	A339	K261	D187	E51
A422	L487	L340	A262	V188	E52
K423	E488	K341	M263	I189	A53
E424	S489	L342	S264	N190	T125
N425		Q347	E265	L191	Q55
R426	L492	L428	R266	A192	S56
P427	M493	V428	L267	S193	L57
G429	D494	G429	R268	S194	S58
L430	L495	A431	V269	L195	L61
E431	D496	E431	I270	R196	I62
V354	W497	P355	L271	A197	
P355	E498	L356	S272	D198	V65
L356	GLY	P357	H273	F199	S66
P357		V363	S277	R200	Q67
V363	P438	P367	D278	R201	E68
P439	P439	A366	A279	D204	Q69
A440	A440	I369	L280	S205	Y70
H441	H441	E370	N381	W206	D71
D442	L443	R371	R282	D210	I72
E444	E444	L372	Q284	R214	N73
T445	T445	R373	R285	I217	Q74
F446	F446	R374	H286	D287	D75
A447	A447	K375	D287	I217	N76
V448	V448	E376	L288	Q221	P77
W449	W449	V377	R289	R224	A81
M452	M452	D378	W290	G225	S82
A453	A453	L291	V292	D226	R83
R454	R454	D379	K293	I227	E84
E455	E455	E380	R294		L85
					R86
					E87

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00296	Depositor
Map size (Å)	464.63998, 464.63998, 464.63998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1616, 1.1616, 1.1616	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/4817	0.32	0/6502
1	B	0.13	0/4817	0.32	0/6502
1	F	0.17	0/4817	0.30	0/6502
1	G	0.11	0/4817	0.27	0/6502
2	C	0.18	0/1592	0.29	0/2164
2	D	0.17	0/1592	0.35	1/2164 (0.0%)
2	H	0.18	0/1592	0.28	0/2164
2	I	0.14	0/1592	0.28	0/2164
3	E	0.16	0/4110	0.32	0/5560
3	J	0.15	0/4110	0.31	0/5560
All	All	0.15	0/33856	0.31	1/45784 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	198	PRO	CA-N-CD	-7.33	101.73	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4735	0	4689	362	0
1	B	4735	0	4689	599	0
1	F	4735	0	4689	363	0
1	G	4735	0	4689	559	0
2	C	1566	0	1605	135	0
2	D	1566	0	1605	125	0
2	H	1566	0	1605	131	0
2	I	1566	0	1605	130	0
3	E	4044	0	4007	493	0
3	J	4044	0	4007	495	0
4	A	27	12	12	1	0
4	B	27	12	12	4	0
4	F	27	12	12	3	0
4	G	27	12	12	2	0
All	All	33400	48	33238	3018	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 45.

All (3018) 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:B:1087:ARG:HG3	3:E:477:ARG:HD2	1.22	1.19
1:B:107:VAL:HG13	1:B:128:TRP:HB3	1.26	1.13
1:A:56:LEU:HD13	1:A:1019:ILE:HD11	1.31	1.12
1:B:982:GLN:HA	1:B:988:GLU:HB2	1.31	1.12
3:E:165:LEU:HD11	3:J:151:VAL:HG13	1.30	1.10
2:D:59:GLY:HA3	3:E:367:PRO:HG2	1.33	1.09
1:G:107:VAL:HG13	1:G:128:TRP:HB3	1.25	1.08
3:E:165:LEU:HB2	3:J:154:LEU:HD22	1.13	1.08
1:G:982:GLN:HA	1:G:988:GLU:HB2	1.35	1.06
3:E:151:VAL:HG13	3:J:165:LEU:HD11	1.33	1.06
1:G:982:GLN:HG2	1:G:984:GLY:H	1.18	1.06
3:E:150:ARG:O	3:E:154:LEU:HD12	1.56	1.05
1:A:1018:ILE:HG21	1:A:1044:LEU:HD13	1.37	1.04
1:B:253:GLU:HA	1:B:256:ARG:HE	1.20	1.03
2:I:59:GLY:HA3	3:J:367:PRO:HG2	1.40	1.03
2:H:230:ILE:HD12	3:J:341:LYS:HB2	1.40	1.03
1:B:982:GLN:HG2	1:B:984:GLY:H	1.19	1.02
3:J:241:THR:HA	3:J:245:ARG:HG3	1.42	1.01
3:E:487:LEU:HG	3:E:492:LEU:HD11	1.42	1.01
3:E:447:ALA:HA	3:E:450:ILE:HD12	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:421:LEU:HD21	3:J:487:LEU:HD23	1.42	1.00
3:E:421:LEU:HD21	3:E:487:LEU:HD23	1.42	1.00
1:F:881:MET:HE1	1:F:894:LEU:HD13	1.39	1.00
1:B:1034:ARG:HH12	1:B:1038:ALA:HB2	1.28	0.99
3:E:241:THR:HA	3:E:245:ARG:HG3	1.41	0.99
1:G:253:GLU:HA	1:G:256:ARG:HE	1.28	0.99
1:F:56:LEU:HD13	1:F:1019:ILE:HD11	1.41	0.98
2:C:45:LEU:HD13	2:C:48:ILE:HD12	1.45	0.98
2:C:53:GLN:NE2	2:D:88:ASP:OD2	1.97	0.98
1:G:211:LEU:HD21	1:G:224:LEU:HD21	1.43	0.98
2:I:209:ILE:HD11	3:J:369:ILE:HG21	1.46	0.97
1:B:42:ILE:HD12	1:B:1055:MET:HE1	1.45	0.97
2:H:45:LEU:HD13	2:H:48:ILE:HD12	1.45	0.97
2:C:230:ILE:HD12	3:E:341:LYS:HB2	1.46	0.97
3:J:176:LEU:O	3:J:177:GLU:HG2	1.63	0.97
3:E:40:LEU:HD22	3:E:48:ILE:HG21	1.47	0.97
1:B:270:GLU:HA	1:B:273:GLN:HE21	1.29	0.96
2:C:124:ARG:HD3	3:E:353:GLU:HG3	1.46	0.96
1:B:211:LEU:HD11	1:B:997:LEU:HD23	1.47	0.96
2:H:73:VAL:HG13	2:H:80:VAL:HG21	1.47	0.95
1:B:87:VAL:HG22	1:B:100:ILE:HG22	1.48	0.95
3:E:196:ARG:HH22	3:E:200:ARG:HD3	1.31	0.95
2:C:226:LEU:HD23	3:E:338:LEU:HD23	1.49	0.95
1:B:874:LEU:HD11	1:B:894:LEU:HG	1.49	0.95
3:E:173:ILE:HG21	3:J:147:PRO:HA	1.48	0.95
1:G:42:ILE:HD12	1:G:1055:MET:HE1	1.48	0.95
3:J:414:ILE:HG12	3:J:452:MET:HE1	1.49	0.94
3:E:414:ILE:HG12	3:E:452:MET:HE1	1.47	0.94
3:E:125:THR:HG22	3:J:246:VAL:HG11	1.48	0.94
1:G:195:PHE:HA	1:G:1014:LEU:HD23	1.49	0.94
3:E:161:LEU:HD22	3:J:158:ILE:HG13	1.48	0.93
1:F:279:LEU:HB2	1:F:786:VAL:HG11	1.49	0.93
3:E:243:GLU:CD	3:J:122:MET:HE1	1.93	0.92
3:J:40:LEU:HD22	3:J:48:ILE:HG21	1.50	0.92
3:J:160:GLU:HA	3:J:163:ARG:HE	1.35	0.92
1:G:87:VAL:HG22	1:G:100:ILE:HG22	1.50	0.92
2:H:89:LEU:HD23	2:H:102:VAL:HG11	1.52	0.92
3:J:487:LEU:HG	3:J:492:LEU:HD11	1.49	0.92
1:B:159:VAL:HG11	1:B:171:MET:SD	2.11	0.91
1:F:1018:ILE:HG21	1:F:1044:LEU:HD13	1.53	0.91
1:G:30:HIS:HB3	1:G:1077:MET:HE2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:157:ARG:HB3	3:J:161:LEU:HD11	1.52	0.90
1:G:270:GLU:HA	1:G:273:GLN:HE21	1.35	0.90
1:B:799:LYS:HD2	1:B:800:ARG:HH12	1.37	0.90
2:H:226:LEU:HD23	3:J:338:LEU:HD23	1.52	0.90
1:G:13:PHE:HB3	1:G:114:LEU:HD23	1.54	0.90
2:I:66:LYS:HE3	2:I:66:LYS:HA	1.53	0.90
3:J:314:ARG:HA	3:J:317:MET:HE2	1.53	0.89
1:F:806:ARG:HH12	1:G:806:ARG:HA	1.36	0.89
2:D:131:LEU:HD13	2:D:226:LEU:HD12	1.54	0.89
3:E:314:ARG:HA	3:E:317:MET:HE2	1.54	0.89
3:E:202:VAL:CG2	3:E:243:GLU:HG2	2.02	0.89
1:B:97:GLN:HB3	1:B:100:ILE:HD11	1.55	0.88
1:B:151:GLN:HE22	1:B:178:LEU:HB2	1.38	0.88
1:G:221:PHE:HB3	1:G:226:LEU:HD22	1.55	0.88
3:J:227:ILE:HD11	3:J:317:MET:HB3	1.54	0.88
1:A:971:SER:OG	1:A:973:ASN:OD1	1.92	0.88
1:F:52:LEU:HD11	1:F:1077:MET:HE1	1.56	0.88
1:A:1056:ARG:HH21	3:E:406:ASN:HA	1.38	0.88
1:A:808:ASP:OD2	1:A:812:LEU:HB2	1.74	0.87
1:F:971:SER:OG	1:F:973:ASN:OD1	1.92	0.87
2:D:66:LYS:HA	2:D:66:LYS:HE3	1.56	0.87
1:F:32:ALA:HB2	1:F:1077:MET:HE2	1.57	0.87
1:G:262:LEU:HB2	1:G:829:LEU:HD23	1.57	0.87
1:F:250:GLN:HA	1:F:253:GLU:HG2	1.55	0.87
1:B:799:LYS:HD2	1:B:800:ARG:NH1	1.90	0.86
1:B:22:ASN:O	1:B:108:THR:OG1	1.93	0.86
2:C:89:LEU:HD23	2:C:102:VAL:HG11	1.55	0.86
3:J:165:LEU:HD12	3:J:168:ALA:HB3	1.56	0.86
1:B:887:GLN:HB3	1:B:888:PRO:HD2	1.57	0.86
3:J:152:ALA:O	3:J:156:ARG:NE	2.09	0.86
3:E:154:LEU:HB3	3:J:161:LEU:CD2	2.05	0.86
1:G:887:GLN:HB3	1:G:888:PRO:HD2	1.56	0.86
1:B:1058:LEU:O	1:B:1062:THR:OG1	1.94	0.85
1:B:812:LEU:HD11	1:B:828:ARG:HG2	1.56	0.85
1:B:248:ILE:HA	1:B:251:GLU:OE1	1.77	0.85
3:J:262:ALA:O	3:J:266:ARG:HG3	1.75	0.85
3:J:430:LEU:HB3	3:J:482:LEU:HD23	1.59	0.85
1:A:834:GLU:HG2	1:A:835:GLU:CG	2.05	0.85
1:A:852:SER:O	1:A:857:THR:OG1	1.95	0.85
1:G:1034:ARG:HH12	1:G:1038:ALA:HB2	1.41	0.85
2:C:45:LEU:H	2:C:45:LEU:HD12	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:165:LEU:HB2	3:J:154:LEU:CD2	2.02	0.85
2:C:68:ASN:O	2:C:72:ILE:HD12	1.77	0.85
1:G:142:LEU:HD21	1:G:180:THR:HG23	1.59	0.85
2:C:69:LEU:O	2:C:73:VAL:HG23	1.76	0.84
1:G:97:GLN:HB3	1:G:100:ILE:HD11	1.57	0.84
3:E:130:SER:O	3:E:134:ARG:HG3	1.78	0.84
2:H:45:LEU:H	2:H:45:LEU:HD12	1.41	0.84
2:D:226:LEU:O	2:D:230:ILE:HG23	1.78	0.84
3:E:38:LYS:NZ	3:E:115:GLU:OE2	2.10	0.84
1:B:247:GLU:O	1:B:251:GLU:HG3	1.77	0.84
3:E:133:GLN:HA	3:J:263:MET:HE2	1.59	0.84
1:F:892:LEU:HD21	1:F:964:VAL:HG13	1.58	0.84
1:F:852:SER:O	1:F:857:THR:OG1	1.95	0.83
1:A:80:LEU:O	1:A:84:VAL:HG23	1.77	0.83
1:A:279:LEU:HB2	1:A:786:VAL:HG11	1.59	0.83
1:A:892:LEU:HD21	1:A:964:VAL:HG13	1.61	0.83
3:E:202:VAL:HG22	3:E:243:GLU:HG2	1.58	0.82
3:J:147:PRO:O	3:J:151:VAL:HG23	1.79	0.82
1:F:1056:ARG:HH21	3:J:406:ASN:HA	1.45	0.82
1:A:242:PHE:O	1:A:246:THR:HG23	1.79	0.82
2:D:168:TYR:OH	2:D:227:ARG:NH2	2.12	0.82
2:H:117:HIS:HB3	2:H:120:VAL:HG12	1.60	0.82
3:E:176:LEU:HD21	3:J:142:ARG:HE	1.43	0.82
1:B:812:LEU:HD23	1:B:824:VAL:HG12	1.61	0.82
2:C:73:VAL:HG13	2:C:80:VAL:HG21	1.61	0.82
1:A:974:VAL:HG21	1:A:977:SER:HB2	1.61	0.82
2:C:129:GLN:NE2	2:C:188:GLN:OE1	2.13	0.82
1:B:785:ARG:NH1	1:B:785:ARG:O	2.13	0.81
3:J:420:LEU:HD22	3:J:437:LEU:HG	1.60	0.81
1:B:1050:THR:HG21	1:B:1053:LYS:O	1.79	0.81
1:F:1022:GLU:OE1	1:F:1022:GLU:N	2.13	0.81
3:E:251:GLN:OE1	3:E:299:SER:HB3	1.79	0.81
1:G:785:ARG:NH1	1:G:785:ARG:O	2.13	0.81
3:E:432:GLU:O	3:E:436:LEU:HG	1.79	0.81
2:H:63:GLU:HB2	2:H:70:TYR:CD1	2.15	0.81
3:E:156:ARG:O	3:E:160:GLU:HG2	1.81	0.81
3:E:63:GLU:OE2	3:J:6:ARG:NE	2.13	0.81
1:B:1031:VAL:O	1:B:1035:ILE:HD12	1.79	0.81
3:E:161:LEU:HD23	3:J:154:LEU:CD2	2.10	0.81
1:F:84:VAL:HG13	1:F:108:THR:CG2	2.11	0.81
3:E:155:ARG:HA	3:E:158:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD13	1:B:171:MET:HE2	1.63	0.80
3:J:414:ILE:O	3:J:418:LEU:HG	1.81	0.80
3:E:246:VAL:HG11	3:J:125:THR:HG22	1.62	0.80
1:A:834:GLU:CD	3:J:241:THR:HB	2.06	0.80
3:E:455:GLU:HG3	3:E:495:ILE:HD12	1.62	0.80
3:E:147:PRO:O	3:E:151:VAL:HG23	1.82	0.80
1:G:1087:ARG:HG3	3:J:477:ARG:HH22	1.47	0.80
3:E:431:ALA:N	3:E:466:GLU:OE1	2.14	0.80
1:G:855:GLY:HA2	1:G:858:GLN:HE21	1.47	0.80
3:E:241:THR:HB	1:F:834:GLU:CD	2.06	0.80
1:B:253:GLU:OE1	1:B:256:ARG:NE	2.15	0.79
3:E:201:ARG:NE	3:E:243:GLU:OE1	2.15	0.79
1:G:142:LEU:HD11	1:G:144:LEU:HD21	1.64	0.79
1:B:39:THR:HG22	1:B:1047:VAL:HG12	1.63	0.79
2:H:53:GLN:NE2	2:I:88:ASP:OD2	2.14	0.79
1:A:1022:GLU:OE1	1:A:1022:GLU:N	2.16	0.79
3:E:110:ALA:O	3:E:114:VAL:HG23	1.82	0.79
3:E:158:ILE:CG1	3:J:161:LEU:HD22	2.12	0.79
1:B:107:VAL:HG21	1:B:160:TYR:HE1	1.47	0.79
3:E:161:LEU:O	3:J:154:LEU:HD21	1.82	0.79
1:A:56:LEU:HD13	1:A:1019:ILE:CD1	2.12	0.79
1:A:795:ILE:CD1	1:B:798:THR:HG21	2.11	0.79
3:J:38:LYS:NZ	3:J:115:GLU:OE2	2.13	0.79
3:J:153:THR:HA	3:J:156:ARG:HD2	1.65	0.79
2:C:117:HIS:HB3	2:C:120:VAL:HG12	1.64	0.79
3:E:431:ALA:O	3:E:435:GLU:HG3	1.82	0.79
1:F:784:GLU:OE1	1:F:784:GLU:N	2.15	0.79
1:G:234:ARG:HB3	1:G:859:LEU:HD12	1.64	0.79
1:F:233:ASP:OD1	1:F:234:ARG:N	2.14	0.79
2:I:223:LEU:HD22	2:I:227:ARG:HH22	1.45	0.79
1:B:253:GLU:HA	1:B:256:ARG:NE	1.95	0.79
2:C:49:ARG:HG2	2:D:86:PRO:O	1.83	0.79
1:B:878:ASN:HD21	1:B:893:ARG:HB2	1.47	0.79
1:A:830:GLN:NE2	1:A:834:GLU:OE1	2.16	0.78
1:F:57:MET:HA	1:F:57:MET:HE2	1.65	0.78
1:A:806:ARG:HH12	1:B:806:ARG:HA	1.48	0.78
1:B:800:ARG:H	1:B:800:ARG:HD2	1.49	0.78
3:E:263:MET:HE3	3:J:133:GLN:OE1	1.83	0.78
1:A:784:GLU:OE1	1:A:784:GLU:N	2.16	0.78
1:B:860:LEU:HD21	1:B:907:LEU:HD11	1.65	0.78
1:F:1056:ARG:HE	3:J:407:GLY:H	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ASN:O	2:D:72:ILE:HG12	1.82	0.78
3:E:161:LEU:HD23	3:J:154:LEU:HD23	1.64	0.78
1:F:135:SER:HB3	1:F:138:ASP:OD2	1.84	0.78
1:G:1050:THR:HG21	1:G:1053:LYS:O	1.83	0.78
1:B:863:ILE:O	1:B:867:VAL:HG23	1.82	0.78
1:B:1087:ARG:HG3	3:E:477:ARG:CD	2.11	0.78
1:B:899:VAL:HG13	1:B:904:LEU:HD11	1.65	0.78
1:G:822:ILE:O	1:G:826:LEU:HG	1.84	0.78
2:I:51:ALA:HA	2:I:69:LEU:HD12	1.66	0.78
1:A:57:MET:HA	1:A:57:MET:HE2	1.66	0.77
2:D:128:GLU:OE1	2:D:128:GLU:N	2.15	0.77
1:F:809:THR:O	1:F:809:THR:HG22	1.85	0.77
1:A:1089:TYR:HB2	3:E:402:TRP:CZ3	2.19	0.77
1:B:168:LEU:HD13	1:B:171:MET:CE	2.14	0.77
1:B:967:MET:HA	1:B:974:VAL:HA	1.66	0.77
1:F:80:LEU:O	1:F:84:VAL:HG23	1.84	0.77
1:G:22:ASN:O	1:G:108:THR:OG1	2.01	0.77
3:J:271:LEU:HD22	3:J:289:ARG:HB2	1.65	0.77
1:G:225:VAL:HG12	1:G:226:LEU:H	1.50	0.77
1:G:247:GLU:O	1:G:251:GLU:HG3	1.85	0.77
2:H:129:GLN:NE2	2:H:188:GLN:OE1	2.17	0.77
1:A:809:THR:HG22	1:A:809:THR:O	1.84	0.77
1:B:822:ILE:O	1:B:826:LEU:HG	1.84	0.77
2:C:143:TRP:HZ2	2:C:152:SER:HB3	1.50	0.77
3:E:267:LEU:HD22	3:J:136:ILE:HD11	1.65	0.77
1:G:158:ASN:O	1:G:162:GLU:HG3	1.85	0.77
1:G:931:LEU:O	1:G:935:VAL:HG12	1.84	0.77
1:B:845:LEU:HA	1:B:848:LEU:HG	1.66	0.77
1:B:1084:GLU:HB2	3:E:478:TRP:CZ3	2.19	0.77
1:B:901:HIS:CE1	1:B:903:SER:HB2	2.20	0.76
3:E:412:VAL:O	3:E:416:GLN:HG2	1.85	0.76
2:H:49:ARG:HG2	2:I:86:PRO:O	1.85	0.76
2:I:61:LEU:HD21	2:I:69:LEU:HB3	1.66	0.76
1:G:881:MET:HE1	1:G:893:ARG:HA	1.67	0.76
2:H:230:ILE:CD1	3:J:341:LYS:HB2	2.15	0.76
3:J:367:PRO:O	3:J:371:ARG:NH1	2.18	0.76
1:B:244:GLY:O	1:B:248:ILE:HD12	1.85	0.76
3:J:432:GLU:O	3:J:436:LEU:HG	1.86	0.76
1:B:181:TYR:HD2	1:B:187:TYR:HB2	1.50	0.76
3:E:137:GLU:O	3:E:141:THR:HG23	1.83	0.76
3:E:177:GLU:HB2	3:E:180:GLN:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:263:MET:HE2	3:J:133:GLN:HA	1.66	0.76
1:G:4:VAL:O	1:G:7:LEU:HG	1.86	0.76
1:B:225:VAL:HG12	1:B:226:LEU:H	1.49	0.76
1:B:982:GLN:HG2	1:B:984:GLY:N	1.99	0.76
3:E:131:THR:HA	3:E:134:ARG:HE	1.51	0.76
1:F:795:ILE:CD1	1:G:798:THR:HG21	2.16	0.76
1:G:19:GLU:HB2	1:G:111:ALA:HB3	1.67	0.76
2:H:68:ASN:O	2:H:72:ILE:HD12	1.86	0.76
1:B:239:ALA:HB1	1:B:939:ARG:HD3	1.66	0.76
3:E:165:LEU:HD11	3:J:151:VAL:CG1	2.13	0.76
1:F:821:ASP:O	1:F:824:VAL:HG22	1.86	0.76
1:G:107:VAL:HG21	1:G:160:TYR:HE1	1.49	0.76
1:G:248:ILE:HA	1:G:251:GLU:OE2	1.84	0.76
1:G:982:GLN:HG2	1:G:984:GLY:N	1.98	0.76
1:B:1057:LEU:HD12	1:B:1058:LEU:N	2.01	0.76
1:B:1085:LEU:HD12	3:E:477:ARG:HD3	1.68	0.76
1:F:53:VAL:HG22	1:F:1019:ILE:HG21	1.68	0.76
1:G:1088:HIS:NE2	1:G:1091:ARG:HB2	2.01	0.76
2:I:168:TYR:OH	2:I:227:ARG:NH2	2.19	0.76
3:J:415:GLN:HA	3:J:418:LEU:HD12	1.67	0.76
1:B:168:LEU:HA	1:B:171:MET:HE2	1.68	0.75
1:B:201:ALA:HB1	1:B:1005:LEU:CD2	2.16	0.75
1:B:818:ASP:OD1	1:B:819:LEU:HD23	1.86	0.75
3:E:133:GLN:OE1	3:J:263:MET:HE3	1.86	0.75
1:G:1057:LEU:HD12	1:G:1058:LEU:N	2.01	0.75
2:D:73:VAL:HG11	2:D:100:LEU:HD13	1.68	0.75
2:I:128:GLU:OE1	2:I:128:GLU:N	2.16	0.75
2:C:55:LEU:HA	2:C:61:LEU:HD11	1.66	0.75
1:A:32:ALA:HB2	1:A:1077:MET:HE2	1.66	0.75
1:B:1076:ASN:HB2	3:E:454:ARG:NH2	2.01	0.75
3:E:159:SER:O	3:E:163:ARG:HG3	1.87	0.75
1:B:1088:HIS:NE2	1:B:1091:ARG:HB2	2.01	0.75
3:J:251:GLN:OE1	3:J:299:SER:HB3	1.87	0.75
1:A:834:GLU:HG2	1:A:835:GLU:HG2	1.67	0.75
1:B:201:ALA:HB1	1:B:1005:LEU:HD23	1.69	0.75
2:H:143:TRP:HZ2	2:H:152:SER:HB3	1.51	0.75
1:B:19:GLU:HB2	1:B:111:ALA:HB3	1.67	0.75
1:B:234:ARG:HB3	1:B:859:LEU:HD12	1.69	0.75
1:G:231:ALA:CB	1:G:863:ILE:HD11	2.18	0.74
3:E:147:PRO:HA	3:J:173:ILE:HG21	1.69	0.74
1:G:805:LYS:HA	1:G:808:ASP:OD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:LEU:HD23	1:G:157:LEU:HD23	1.70	0.74
3:E:161:LEU:HD11	3:J:157:ARG:HB3	1.69	0.74
2:C:156:ILE:HD11	2:C:161:LEU:HD11	1.70	0.74
3:E:165:LEU:CB	3:J:154:LEU:HD22	2.07	0.74
1:G:105:LYS:CE	1:G:130:ASP:HA	2.17	0.74
2:I:175:GLU:HA	2:I:178:GLU:OE2	1.88	0.74
1:A:787:LYS:HE2	1:A:787:LYS:HA	1.70	0.74
1:B:819:LEU:O	1:B:822:ILE:HG12	1.87	0.74
2:D:59:GLY:CA	3:E:367:PRO:HG2	2.16	0.74
1:G:818:ASP:OD1	1:G:819:LEU:HD23	1.87	0.74
2:H:55:LEU:HD13	2:H:61:LEU:HD12	1.69	0.74
2:H:63:GLU:HB2	2:H:70:TYR:HD1	1.53	0.74
3:E:246:VAL:CG1	3:J:125:THR:HG22	2.17	0.74
3:E:417:THR:O	3:E:421:LEU:HD12	1.87	0.74
1:G:967:MET:HA	1:G:974:VAL:HA	1.69	0.74
1:B:159:VAL:HG13	1:B:167:LEU:HG	1.69	0.74
3:E:419:GLN:HG3	3:E:423:LYS:HE2	1.69	0.74
1:F:95:GLU:HA	1:F:99:HIS:NE2	2.03	0.74
1:A:95:GLU:HA	1:A:99:HIS:NE2	2.03	0.74
2:C:124:ARG:HD3	3:E:353:GLU:CG	2.17	0.74
3:E:367:PRO:O	3:E:371:ARG:NH1	2.21	0.74
3:E:161:LEU:HD22	3:J:158:ILE:CG1	2.18	0.73
1:F:85:ARG:NH2	1:F:133:SER:O	2.21	0.73
1:A:172:GLU:HG3	1:A:180:THR:HG23	1.70	0.73
1:B:17:ARG:HH12	1:B:31:GLN:HB2	1.53	0.73
3:E:151:VAL:HA	3:J:165:LEU:HD13	1.70	0.73
1:A:85:ARG:NH2	1:A:133:SER:O	2.20	0.73
1:B:200:ASN:OD1	1:B:201:ALA:N	2.21	0.73
1:B:246:THR:HG23	1:B:928:TYR:OH	1.87	0.73
1:B:258:GLN:O	1:B:262:LEU:HD13	1.87	0.73
2:D:63:GLU:HB2	2:D:70:TYR:CD2	2.23	0.73
3:E:125:THR:HG22	3:J:246:VAL:CG1	2.18	0.73
1:G:255:ALA:HB2	1:G:840:LYS:NZ	2.03	0.73
1:A:892:LEU:HD23	1:A:893:ARG:N	2.04	0.73
1:B:105:LYS:CE	1:B:130:ASP:HA	2.19	0.73
1:B:116:ARG:HH12	1:B:117:GLU:HB3	1.53	0.73
3:E:165:LEU:HD23	3:J:155:ARG:CD	2.17	0.73
3:E:129:LEU:O	3:E:133:GLN:HG2	1.89	0.73
1:G:141:ARG:HH12	1:G:184:LYS:H	1.37	0.73
1:G:1050:THR:HG23	1:G:1051:PRO:HD2	1.71	0.73
3:J:114:VAL:O	3:J:117:LEU:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:MET:CE	1:B:206:ASN:HA	2.18	0.73
2:H:44:THR:HG23	2:I:85:GLU:OE1	1.89	0.73
1:B:1034:ARG:NH1	1:B:1038:ALA:HB2	2.01	0.73
1:A:250:GLN:HA	1:A:253:GLU:HG2	1.71	0.73
3:E:241:THR:OG1	3:E:245:ARG:NH1	2.22	0.73
1:F:1056:ARG:HH21	3:J:406:ASN:CA	2.02	0.73
2:H:124:ARG:NE	3:J:353:GLU:OE1	2.19	0.73
3:E:158:ILE:HG23	3:J:158:ILE:HG23	1.71	0.73
1:B:1050:THR:HG23	1:B:1051:PRO:HD2	1.71	0.72
1:F:1089:TYR:HB2	3:J:402:TRP:CZ3	2.24	0.72
3:J:233:ASN:HD21	3:J:235:GLN:HB2	1.54	0.72
1:A:897:LYS:HG2	1:A:898:LYS:H	1.54	0.72
1:B:881:MET:HE3	1:B:892:LEU:O	1.90	0.72
3:E:165:LEU:CD1	3:J:151:VAL:HA	2.20	0.72
3:E:465:ARG:HD3	3:E:481:ASN:HD21	1.53	0.72
1:G:17:ARG:HH12	1:G:31:GLN:HB2	1.53	0.72
1:G:899:VAL:HG12	1:G:959:ARG:O	1.89	0.72
1:B:234:ARG:HA	1:B:237:GLU:OE1	1.90	0.72
3:E:161:LEU:HD21	3:J:154:LEU:O	1.89	0.72
3:E:266:ARG:HB3	3:J:140:GLU:OE2	1.89	0.72
1:G:211:LEU:HD21	1:G:224:LEU:CD2	2.19	0.72
1:A:856:VAL:HG21	1:A:931:LEU:HD11	1.70	0.72
1:A:1036:ILE:HG21	1:A:1061:HIS:HB3	1.72	0.72
1:B:211:LEU:HD11	1:B:997:LEU:CD2	2.19	0.72
1:G:22:ASN:HA	1:G:102:ARG:NH2	2.03	0.72
3:E:147:PRO:HG3	3:J:173:ILE:HD13	1.70	0.72
1:G:120:GLN:HE22	1:G:122:ARG:HB2	1.53	0.72
2:I:59:GLY:CA	3:J:367:PRO:HG2	2.18	0.72
1:A:834:GLU:HG2	1:A:835:GLU:HG3	1.72	0.72
1:B:158:ASN:O	1:B:162:GLU:HG3	1.90	0.72
1:F:884:VAL:HG13	1:F:1041:GLU:OE1	1.89	0.72
2:I:209:ILE:HD11	3:J:369:ILE:CG2	2.18	0.72
3:J:160:GLU:HA	3:J:163:ARG:NE	2.04	0.72
3:J:243:GLU:OE1	3:J:243:GLU:N	2.22	0.72
1:A:128:TRP:CE2	1:A:140:LYS:HB2	2.25	0.72
1:A:884:VAL:HG13	1:A:1041:GLU:OE1	1.89	0.72
2:D:175:GLU:HA	2:D:178:GLU:OE2	1.89	0.72
3:E:151:VAL:O	3:E:155:ARG:HG3	1.88	0.72
2:I:131:LEU:HD13	2:I:226:LEU:CD1	2.20	0.72
3:J:146:ASN:ND2	3:J:149:ASN:OD1	2.23	0.72
1:A:850:ARG:NE	3:J:14:SER:OG	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:SER:OG	3:E:354:VAL:HG21	1.88	0.72
1:F:1057:LEU:HD12	1:F:1057:LEU:O	1.90	0.72
1:G:80:LEU:O	1:G:84:VAL:HG22	1.90	0.72
1:G:146:SER:HB2	1:G:178:LEU:HD21	1.71	0.72
2:I:226:LEU:O	2:I:230:ILE:HG23	1.88	0.72
1:A:1039:LEU:HD21	1:A:1046:ALA:HB2	1.70	0.72
1:B:144:LEU:HB2	1:B:156:TRP:CZ3	2.25	0.72
1:B:874:LEU:HD11	1:B:894:LEU:CG	2.19	0.72
1:F:806:ARG:NH2	1:G:806:ARG:HB2	2.04	0.72
1:B:855:GLY:HA2	1:B:858:GLN:HE21	1.54	0.71
3:J:261:LYS:HE2	3:J:261:LYS:H	1.54	0.71
1:B:982:GLN:HA	1:B:988:GLU:CB	2.17	0.71
1:G:57:MET:CE	1:G:206:ASN:HA	2.20	0.71
1:G:234:ARG:HA	1:G:237:GLU:OE1	1.90	0.71
1:G:876:GLU:HB3	1:G:1003:TYR:OH	1.91	0.71
1:B:164:GLY:O	1:B:168:LEU:HD23	1.90	0.71
3:E:62:ILE:O	3:E:65:VAL:HG13	1.90	0.71
3:E:261:LYS:HE2	3:E:261:LYS:H	1.54	0.71
3:J:455:GLU:HG3	3:J:495:ILE:HD12	1.71	0.71
1:B:815:ALA:HB1	1:B:821:ASP:OD2	1.90	0.71
1:G:815:ALA:HB1	1:G:821:ASP:OD2	1.91	0.71
3:J:417:THR:O	3:J:421:LEU:HD12	1.89	0.71
1:F:1036:ILE:HG21	1:F:1061:HIS:HB3	1.73	0.71
1:F:893:ARG:HG2	1:F:894:LEU:H	1.56	0.71
1:G:812:LEU:HD23	1:G:824:VAL:HG12	1.72	0.71
1:A:834:GLU:OE2	3:J:241:THR:HB	1.91	0.71
3:E:111:ILE:O	3:E:115:GLU:HG3	1.90	0.71
3:E:154:LEU:HB3	3:J:161:LEU:HD21	1.71	0.71
3:E:470:LEU:HD13	3:E:471:SER:N	2.05	0.71
1:A:162:GLU:HG2	1:A:167:LEU:HD23	1.73	0.71
1:B:242:PHE:CE2	1:B:932:GLN:HA	2.25	0.71
1:B:965:SER:HB3	1:B:974:VAL:HG21	1.73	0.71
2:H:44:THR:O	2:H:49:ARG:NH2	2.23	0.71
3:E:229:GLU:HB2	1:F:267:LEU:HG	1.73	0.71
1:G:899:VAL:HG13	1:G:904:LEU:HD11	1.71	0.71
1:A:52:LEU:HD21	1:A:1077:MET:HE1	1.72	0.71
1:B:69:ALA:HB1	1:B:1022:GLU:HG3	1.73	0.71
2:C:138:GLN:NE2	1:F:919:PHE:O	2.24	0.71
3:E:146:ASN:ND2	3:E:149:ASN:OD1	2.24	0.71
1:F:84:VAL:HG13	1:F:108:THR:HG21	1.70	0.71
1:F:881:MET:HE1	1:F:894:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1056:ARG:NE	3:J:407:GLY:H	1.88	0.71
1:F:1083:GLU:O	1:F:1086:GLU:HG2	1.91	0.71
1:G:893:ARG:HD3	1:G:967:MET:SD	2.31	0.71
1:B:925:GLU:OE1	1:B:925:GLU:N	2.24	0.70
3:J:233:ASN:OD1	3:J:235:GLN:N	2.24	0.70
1:A:162:GLU:HG2	1:A:167:LEU:CD2	2.21	0.70
1:A:1018:ILE:CG2	1:A:1044:LEU:HD13	2.19	0.70
1:B:269:TRP:CD2	1:B:822:ILE:HG21	2.26	0.70
1:G:1084:GLU:HB2	3:J:478:TRP:CZ3	2.26	0.70
2:C:230:ILE:CD1	3:E:341:LYS:HB2	2.20	0.70
3:E:114:VAL:O	3:E:117:LEU:HB2	1.91	0.70
1:G:200:ASN:OD1	1:G:201:ALA:N	2.24	0.70
2:H:117:HIS:HB3	2:H:120:VAL:CG1	2.22	0.70
2:I:74:LEU:O	2:I:77:PRO:HD3	1.90	0.70
1:A:233:ASP:OD1	1:A:234:ARG:N	2.24	0.70
1:B:151:GLN:NE2	1:B:178:LEU:HB2	2.06	0.70
3:E:318:LYS:O	3:E:319:THR:OG1	2.09	0.70
3:E:414:ILE:CG1	3:E:452:MET:HE1	2.21	0.70
2:H:156:ILE:HD11	2:H:161:LEU:HD11	1.73	0.70
2:C:70:TYR:HE2	2:C:100:LEU:HD21	1.57	0.70
1:G:819:LEU:O	1:G:822:ILE:HG12	1.90	0.70
1:G:909:LYS:HA	1:G:912:ARG:NH1	2.07	0.70
1:G:1034:ARG:NH1	1:G:1038:ALA:HB2	2.05	0.70
1:G:1054:GLU:HG2	1:G:1057:LEU:HG	1.74	0.70
3:J:448:VAL:O	3:J:452:MET:HG2	1.92	0.70
1:B:885:ASP:OD2	1:B:889:ASP:HA	1.92	0.70
1:B:896:THR:OG1	1:B:960:LEU:HD13	1.92	0.70
1:B:899:VAL:HG12	1:B:959:ARG:O	1.90	0.70
3:E:310:GLU:OE2	3:E:314:ARG:NH2	2.21	0.70
1:F:56:LEU:HD13	1:F:1019:ILE:CD1	2.19	0.70
3:J:295:LEU:O	3:J:299:SER:OG	2.10	0.70
1:G:909:LYS:HA	1:G:912:ARG:HH12	1.57	0.70
1:B:866:GLU:O	1:B:870:ILE:HG13	1.92	0.70
1:F:57:MET:HE1	1:F:205:LEU:HD22	1.74	0.70
1:B:268:SER:HB3	1:B:797:LEU:HD22	1.73	0.70
3:E:233:ASN:HD21	3:E:235:GLN:HB2	1.56	0.70
3:E:158:ILE:HG13	3:J:161:LEU:HD22	1.73	0.69
1:F:897:LYS:HG2	1:F:898:LYS:H	1.55	0.69
1:G:69:ALA:HB1	1:G:1022:GLU:HG3	1.73	0.69
1:G:258:GLN:O	1:G:262:LEU:HD13	1.92	0.69
2:H:55:LEU:HB2	2:H:61:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD21	1:A:1077:MET:CE	2.21	0.69
1:B:948:LEU:HD12	1:B:949:GLY:N	2.07	0.69
1:B:1026:ARG:H	1:B:1026:ARG:HD3	1.57	0.69
1:G:244:GLY:O	1:G:248:ILE:HD12	1.91	0.69
1:G:830:GLN:NE2	1:G:834:GLU:OE2	2.24	0.69
2:H:96:ILE:HD12	3:J:319:THR:HB	1.74	0.69
1:B:20:LEU:HD12	1:B:26:PHE:HD1	1.56	0.69
1:B:146:SER:HB2	1:B:178:LEU:HD23	1.74	0.69
1:B:167:LEU:HD12	1:B:167:LEU:O	1.91	0.69
1:B:269:TRP:O	1:B:273:GLN:HG3	1.92	0.69
3:E:233:ASN:OD1	3:E:235:GLN:N	2.26	0.69
1:G:195:PHE:HA	1:G:1014:LEU:CD2	2.22	0.69
1:A:806:ARG:NH2	1:B:806:ARG:HB2	2.08	0.69
1:B:909:LYS:HA	1:B:912:ARG:NH1	2.07	0.69
1:B:238:VAL:CG2	1:B:856:VAL:HG22	2.22	0.69
2:D:138:GLN:O	2:D:141:VAL:HG12	1.91	0.69
3:E:421:LEU:HD21	3:E:487:LEU:CD2	2.22	0.69
1:G:107:VAL:CG1	1:G:128:TRP:HB3	2.14	0.69
1:G:261:SER:O	1:G:264:PRO:HD2	1.92	0.69
1:G:1035:ILE:H	1:G:1035:ILE:HD12	1.58	0.69
2:I:66:LYS:HE3	2:I:66:LYS:CA	2.22	0.69
2:I:226:LEU:CD2	3:J:385:LEU:HD21	2.23	0.69
3:J:310:GLU:OE2	3:J:314:ARG:NH2	2.24	0.69
3:J:466:GLU:OE2	3:J:484:THR:HA	1.92	0.69
2:C:52:THR:HG21	2:C:83:ILE:HG21	1.74	0.69
3:E:165:LEU:HD12	3:E:168:ALA:HB3	1.75	0.69
1:A:906:THR:HA	1:A:909:LYS:HD3	1.75	0.69
1:B:32:ALA:HB1	1:B:1066:ILE:HD13	1.73	0.69
1:B:234:ARG:O	1:B:237:GLU:HG2	1.93	0.69
1:F:1018:ILE:CG2	1:F:1044:LEU:HD13	2.22	0.69
1:G:50:THR:HG22	1:G:1021:ASP:OD1	1.92	0.69
1:G:816:GLY:N	1:G:821:ASP:OD2	2.26	0.69
2:I:131:LEU:HD13	2:I:226:LEU:HD12	1.74	0.69
1:A:273:GLN:O	1:A:276:GLU:HG3	1.92	0.69
3:E:263:MET:O	3:E:267:LEU:HD23	1.93	0.69
1:G:982:GLN:HA	1:G:988:GLU:CB	2.21	0.69
2:I:78:GLU:OE1	2:I:78:GLU:N	2.26	0.69
2:I:144:GLU:OE1	2:I:150:GLY:N	2.26	0.69
3:J:110:ALA:O	3:J:114:VAL:HG23	1.93	0.69
3:J:137:GLU:O	3:J:141:THR:HG23	1.92	0.69
1:A:81:ILE:HD13	1:A:139:MET:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:PHE:HB3	1:B:114:LEU:HD23	1.74	0.69
1:B:113:THR:HG22	1:B:122:ARG:HG3	1.74	0.69
3:E:321:LEU:HA	3:E:324:GLU:OE1	1.93	0.69
3:J:129:LEU:O	3:J:133:GLN:HG2	1.93	0.69
1:G:17:ARG:NH1	1:G:31:GLN:HB2	2.07	0.69
1:G:234:ARG:O	1:G:237:GLU:HG2	1.92	0.69
3:J:159:SER:O	3:J:163:ARG:HG3	1.92	0.69
1:B:800:ARG:HD2	1:B:800:ARG:N	2.07	0.68
1:B:1054:GLU:HG2	1:B:1057:LEU:HG	1.73	0.68
2:C:44:THR:HG23	2:D:85:GLU:OE1	1.93	0.68
3:E:14:SER:O	3:E:18:GLN:HG3	1.93	0.68
3:E:154:LEU:O	3:E:158:ILE:HG13	1.93	0.68
1:G:272:TYR:HE1	1:G:790:LEU:HD21	1.58	0.68
2:H:119:LEU:HD23	3:J:363:VAL:HG21	1.75	0.68
2:H:158:ILE:HD11	2:H:204:ILE:CG2	2.23	0.68
1:B:876:GLU:HB3	1:B:1003:TYR:OH	1.93	0.68
2:D:131:LEU:HD13	2:D:226:LEU:CD1	2.22	0.68
3:E:347:GLN:O	3:E:351:LYS:HG2	1.93	0.68
1:A:795:ILE:HD12	1:B:798:THR:HG21	1.74	0.68
2:C:137:ARG:HG3	3:E:332:LEU:HD11	1.75	0.68
2:D:209:ILE:HD11	3:E:369:ILE:HG21	1.75	0.68
3:E:64:HIS:O	3:E:72:ILE:HD12	1.93	0.68
1:G:869:VAL:HA	1:G:872:GLU:HG2	1.75	0.68
1:G:896:THR:OG1	1:G:960:LEU:HD13	1.93	0.68
1:A:135:SER:HB3	1:A:138:ASP:OD1	1.92	0.68
1:A:272:TYR:HA	1:A:793:LEU:HD23	1.73	0.68
1:B:901:HIS:HE1	1:B:903:SER:HB2	1.56	0.68
1:F:1087:ARG:HB3	1:F:1091:ARG:NH2	2.09	0.68
1:G:1088:HIS:CE1	1:G:1091:ARG:HB2	2.29	0.68
2:C:44:THR:O	2:C:49:ARG:NH2	2.25	0.68
1:F:142:LEU:CD2	1:F:168:LEU:HD13	2.24	0.68
1:F:795:ILE:HD11	1:G:794:ASN:OD1	1.93	0.68
1:G:275:GLN:NE2	1:G:786:VAL:O	2.25	0.68
1:G:800:ARG:HD2	1:G:800:ARG:N	2.07	0.68
2:I:138:GLN:O	2:I:141:VAL:HG12	1.92	0.68
1:A:963:ALA:HB1	1:A:979:THR:HA	1.75	0.68
3:E:39:THR:OG1	3:J:8:ARG:NH2	2.27	0.68
1:F:795:ILE:HD12	1:G:798:THR:HG21	1.74	0.68
2:H:89:LEU:HD23	2:H:102:VAL:CG1	2.23	0.68
3:E:154:LEU:HB3	3:J:161:LEU:HD23	1.74	0.68
1:F:787:LYS:HA	1:F:787:LYS:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HG	3:J:229:GLU:HB2	1.76	0.68
1:B:1077:MET:O	3:E:454:ARG:NH2	2.26	0.68
3:E:413:LEU:HD11	3:E:449:TRP:HE1	1.58	0.68
1:G:228:ASP:HA	1:G:957:ARG:CZ	2.24	0.68
1:G:801:MET:HG2	1:G:825:TYR:CE2	2.28	0.68
3:J:257:SER:HA	3:J:261:LYS:NZ	2.09	0.68
2:D:144:GLU:OE1	2:D:150:GLY:N	2.23	0.68
1:F:128:TRP:CE2	1:F:140:LYS:HB2	2.29	0.68
3:J:414:ILE:CG1	3:J:452:MET:HE1	2.21	0.68
1:B:228:ASP:HA	1:B:957:ARG:CZ	2.24	0.68
2:C:63:GLU:HB2	2:C:70:TYR:CD1	2.29	0.68
3:E:160:GLU:HA	3:E:163:ARG:HE	1.57	0.68
1:G:164:GLY:O	1:G:168:LEU:HD23	1.94	0.68
1:A:850:ARG:O	1:A:854:ASP:HB2	1.93	0.67
3:E:158:ILE:CG2	3:J:158:ILE:HG23	2.25	0.67
1:G:1076:ASN:HB2	3:J:454:ARG:NH2	2.09	0.67
1:B:262:LEU:CB	1:B:829:LEU:HD23	2.24	0.67
1:B:933:VAL:HG12	1:B:937:GLN:NE2	2.09	0.67
1:B:1038:ALA:HA	1:B:1041:GLU:OE1	1.94	0.67
2:C:117:HIS:HB3	2:C:120:VAL:CG1	2.24	0.67
1:F:892:LEU:HD23	1:F:893:ARG:N	2.09	0.67
2:H:130:SER:OG	3:J:354:VAL:HG21	1.94	0.67
1:B:107:VAL:HG21	1:B:160:TYR:CE1	2.27	0.67
3:E:418:LEU:HD12	3:E:419:GLN:N	2.09	0.67
1:G:965:SER:HB3	1:G:974:VAL:HG21	1.77	0.67
3:J:430:LEU:HG	3:J:485:THR:HG21	1.75	0.67
1:B:794:ASN:O	1:B:798:THR:HG23	1.94	0.67
3:E:226:ASP:OD1	3:E:230:ARG:NH2	2.27	0.67
1:F:808:ASP:OD2	1:F:812:LEU:HB2	1.93	0.67
1:F:836:ALA:O	1:F:840:LYS:HG2	1.94	0.67
1:G:983:GLY:H	1:G:988:GLU:H	1.43	0.67
2:H:74:LEU:O	2:H:77:PRO:HD3	1.93	0.67
2:I:172:PRO:HG2	2:I:178:GLU:HG3	1.75	0.67
3:E:145:PRO:O	3:J:173:ILE:HD12	1.94	0.67
3:E:202:VAL:HG23	3:E:243:GLU:HG2	1.76	0.67
2:I:47:LYS:HA	2:I:47:LYS:HE2	1.77	0.67
2:I:141:VAL:O	2:I:145:GLN:HG2	1.92	0.67
1:B:68:LEU:HB3	1:B:210:GLY:HA3	1.76	0.67
3:E:34:LEU:HD13	3:E:114:VAL:HG21	1.75	0.67
3:E:151:VAL:HG13	3:J:165:LEU:CD1	2.18	0.67
1:F:81:ILE:HD13	1:F:139:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:GLU:HA	1:G:250:GLN:OE1	1.95	0.67
1:G:253:GLU:HA	1:G:256:ARG:NE	2.07	0.67
1:G:885:ASP:OD1	1:G:889:ASP:HA	1.94	0.67
1:G:116:ARG:HH12	1:G:117:GLU:HB3	1.58	0.67
3:J:14:SER:O	3:J:18:GLN:HG3	1.94	0.67
3:J:92:ARG:HH11	3:J:92:ARG:HG3	1.60	0.67
1:A:17:ARG:NH2	1:A:31:GLN:OE1	2.28	0.67
3:E:461:ILE:HD12	3:E:464:GLN:HB2	1.77	0.67
1:A:836:ALA:O	1:A:840:LYS:HG2	1.94	0.67
1:B:17:ARG:NH1	1:B:31:GLN:HB2	2.09	0.67
1:B:801:MET:HE2	1:B:817:ALA:HA	1.77	0.67
2:C:89:LEU:HD23	2:C:102:VAL:CG1	2.23	0.67
1:G:91:GLY:HA3	1:G:99:HIS:CG	2.29	0.67
1:G:211:LEU:HD13	1:G:212:LYS:O	1.95	0.67
1:G:231:ALA:HB2	1:G:863:ILE:HD11	1.76	0.67
3:J:347:GLN:O	3:J:351:LYS:HG2	1.95	0.67
1:B:259:GLN:NE2	1:B:263:GLN:OE1	2.28	0.67
1:B:1059:ARG:HG3	3:E:443:LEU:HD22	1.77	0.67
2:D:172:PRO:HG2	2:D:178:GLU:HG3	1.76	0.67
3:E:165:LEU:HD13	3:J:151:VAL:HA	1.77	0.67
3:E:408:LEU:HB2	3:E:441:HIS:HD2	1.60	0.67
1:F:128:TRP:CG	1:F:160:TYR:HH	2.13	0.67
2:H:85:GLU:O	2:I:43:ARG:NH2	2.28	0.67
1:A:64:PRO:HA	1:A:206:ASN:ND2	2.09	0.66
1:B:91:GLY:HA3	1:B:99:HIS:CG	2.30	0.66
1:B:814:GLU:OE1	1:B:814:GLU:N	2.28	0.66
1:B:983:GLY:H	1:B:988:GLU:H	1.43	0.66
2:D:78:GLU:N	2:D:78:GLU:OE1	2.28	0.66
1:A:200:ASN:O	1:A:203:THR:HG22	1.96	0.66
1:A:812:LEU:HG	1:A:825:TYR:CE1	2.30	0.66
1:B:262:LEU:HB2	1:B:829:LEU:HD23	1.78	0.66
1:B:270:GLU:HA	1:B:273:GLN:NE2	2.07	0.66
1:G:143:TRP:O	1:G:144:LEU:HD23	1.95	0.66
1:G:238:VAL:CG2	1:G:856:VAL:HG22	2.25	0.66
2:C:106:LEU:HB2	2:C:110:PRO:CD	2.25	0.66
1:G:866:GLU:O	1:G:870:ILE:HG13	1.96	0.66
1:G:948:LEU:HD12	1:G:949:GLY:N	2.09	0.66
1:G:1026:ARG:H	1:G:1026:ARG:HD3	1.59	0.66
2:C:96:ILE:HD12	3:E:319:THR:HB	1.78	0.66
1:G:105:LYS:HE3	1:G:130:ASP:HA	1.78	0.66
1:G:189:ALA:HA	1:G:192:ARG:HH12	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:GLN:HA	1:G:253:GLU:HG2	1.76	0.66
1:G:794:ASN:O	1:G:798:THR:HG23	1.95	0.66
1:B:275:GLN:NE2	1:B:786:VAL:O	2.29	0.66
3:E:92:ARG:HH11	3:E:92:ARG:HG3	1.60	0.66
3:E:217:ILE:HG23	3:E:227:ILE:HD11	1.77	0.66
1:F:17:ARG:NH2	1:F:31:GLN:OE1	2.29	0.66
1:B:1032:ALA:HA	1:B:1035:ILE:CD1	2.24	0.66
1:B:1088:HIS:CE1	1:B:1091:ARG:HB2	2.30	0.66
3:E:224:ARG:O	3:E:228:VAL:HG22	1.94	0.66
2:H:106:LEU:HB2	2:H:110:PRO:CD	2.26	0.66
3:J:226:ASP:OD1	3:J:230:ARG:NH2	2.28	0.66
3:E:266:ARG:HB3	3:J:140:GLU:CD	2.20	0.66
1:G:860:LEU:HD21	1:G:907:LEU:HD11	1.76	0.66
1:B:816:GLY:N	1:B:821:ASP:OD2	2.29	0.66
2:C:230:ILE:O	2:C:233:GLN:HG3	1.96	0.66
3:J:156:ARG:O	3:J:160:GLU:HG2	1.96	0.66
1:A:279:LEU:HB2	1:A:786:VAL:CG1	2.25	0.66
3:E:198:ASP:HB2	3:J:124:SER:HB3	1.77	0.66
3:E:257:SER:HA	3:E:261:LYS:NZ	2.11	0.66
1:G:123:LEU:HD21	1:G:191:LEU:HD11	1.78	0.66
2:I:121:ARG:O	3:J:371:ARG:HD2	1.96	0.66
1:A:801:MET:HE2	1:A:822:ILE:HD11	1.77	0.66
1:B:234:ARG:HH21	1:B:859:LEU:HA	1.61	0.66
3:E:176:LEU:HD23	3:J:142:ARG:HH21	1.60	0.66
1:G:143:TRP:C	1:G:144:LEU:HD23	2.20	0.66
1:G:269:TRP:CD2	1:G:822:ILE:HG21	2.31	0.66
3:J:196:ARG:HG2	3:J:199:PHE:HD2	1.59	0.66
3:J:431:ALA:O	3:J:435:GLU:HG3	1.96	0.66
1:A:832:LEU:HD23	1:A:836:ALA:HB3	1.77	0.65
3:J:408:LEU:HB2	3:J:441:HIS:HD2	1.60	0.65
1:B:889:ASP:O	1:B:890:ARG:HD2	1.96	0.65
3:E:448:VAL:O	3:E:452:MET:HG2	1.95	0.65
1:G:113:THR:HG22	1:G:122:ARG:HG3	1.78	0.65
1:G:142:LEU:HD21	1:G:180:THR:CG2	2.26	0.65
1:G:793:LEU:O	1:G:797:LEU:HD23	1.96	0.65
1:G:1020:LEU:CD1	1:G:1023:ALA:HA	2.26	0.65
1:B:231:ALA:CB	1:B:863:ILE:HD11	2.26	0.65
3:E:134:ARG:HH11	3:J:138:ASN:HD22	1.44	0.65
1:G:209:ALA:HA	1:G:1020:LEU:HA	1.76	0.65
1:G:269:TRP:O	1:G:273:GLN:HG3	1.96	0.65
1:G:982:GLN:HG3	1:G:986:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:LEU:HD23	3:J:363:VAL:CG2	2.26	0.65
2:I:68:ASN:O	2:I:72:ILE:HG12	1.95	0.65
1:B:121:VAL:HG21	1:B:194:PHE:CE1	2.32	0.65
1:B:255:ALA:HB2	1:B:840:LYS:NZ	2.11	0.65
1:B:909:LYS:HA	1:B:912:ARG:HH12	1.59	0.65
1:B:1087:ARG:CG	3:E:477:ARG:HD2	2.15	0.65
3:J:122:MET:HB3	3:J:125:THR:CG2	2.27	0.65
2:I:92:GLY:HA3	2:I:101:TYR:CE1	2.31	0.65
3:J:139:LEU:O	3:J:143:LEU:HB2	1.96	0.65
2:C:115:TRP:HB2	2:C:124:ARG:NH1	2.12	0.65
3:E:314:ARG:HA	3:E:317:MET:CE	2.26	0.65
1:G:211:LEU:CD2	1:G:224:LEU:HD21	2.22	0.65
1:G:814:GLU:OE1	1:G:814:GLU:N	2.28	0.65
1:A:782:GLU:HG2	1:A:783:ILE:H	1.61	0.65
1:B:18:ILE:HD11	1:B:56:LEU:HD22	1.79	0.65
1:B:975:ILE:HG22	1:B:976:GLU:CD	2.22	0.65
3:E:236:ASP:OD2	3:E:306:ARG:NH1	2.30	0.65
2:I:51:ALA:CA	2:I:69:LEU:HD12	2.26	0.65
3:J:127:SER:OG	3:J:187:ASP:OD1	2.13	0.65
3:J:446:PHE:CE1	3:J:482:LEU:HD21	2.32	0.65
1:A:795:ILE:HD11	1:B:794:ASN:OD1	1.97	0.65
1:A:834:GLU:O	1:A:838:PRO:HG2	1.97	0.65
1:B:141:ARG:HH12	1:B:184:LYS:H	1.44	0.65
1:B:875:ASN:O	1:B:879:GLU:HG2	1.97	0.65
1:B:903:SER:O	1:B:906:THR:HG22	1.96	0.65
1:G:891:TYR:CZ	1:G:967:MET:HB2	2.32	0.65
1:G:891:TYR:HD2	1:G:969:ARG:HD3	1.60	0.65
1:A:142:LEU:HD22	1:A:168:LEU:HD13	1.79	0.65
1:A:217:ILE:O	1:A:220:ILE:HG12	1.97	0.65
1:A:274:LYS:HE2	1:A:277:ARG:HE	1.62	0.65
1:B:878:ASN:ND2	1:B:893:ARG:HB2	2.12	0.65
2:C:74:LEU:O	2:C:77:PRO:HD3	1.97	0.65
3:E:157:ARG:CB	3:J:161:LEU:HD11	2.24	0.65
3:E:160:GLU:HA	3:E:163:ARG:NE	2.12	0.65
1:G:1087:ARG:CG	3:J:477:ARG:HH22	2.09	0.65
1:B:801:MET:CE	1:B:817:ALA:HA	2.27	0.64
2:C:107:ASP:OD2	2:D:43:ARG:HD3	1.97	0.64
1:F:84:VAL:HG13	1:F:108:THR:HG22	1.79	0.64
1:G:938:LEU:HD22	1:G:954:LEU:HD11	1.78	0.64
1:G:975:ILE:HG22	1:G:976:GLU:CD	2.22	0.64
1:G:1038:ALA:HA	1:G:1041:GLU:OE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:LEU:CD1	1:B:1023:ALA:HA	2.28	0.64
1:G:30:HIS:CB	1:G:1077:MET:HE2	2.27	0.64
1:G:111:ALA:CB	1:G:153:LEU:HD12	2.27	0.64
1:B:982:GLN:HG3	1:B:986:GLY:H	1.61	0.64
2:D:63:GLU:HB2	2:D:70:TYR:HD2	1.60	0.64
2:D:74:LEU:O	2:D:77:PRO:HD3	1.97	0.64
3:E:273:HIS:CD2	3:J:143:LEU:HD21	2.33	0.64
1:F:121:VAL:HG21	1:F:194:PHE:CZ	2.32	0.64
1:F:859:LEU:HD23	1:F:938:LEU:HD21	1.79	0.64
3:J:150:ARG:O	3:J:154:LEU:HB2	1.98	0.64
3:J:421:LEU:HD21	3:J:487:LEU:CD2	2.20	0.64
3:J:462:ASP:OD1	3:J:483:PRO:HB3	1.98	0.64
3:J:469:GLU:HB3	3:J:477:ARG:HD2	1.78	0.64
1:F:273:GLN:O	1:F:276:GLU:HG3	1.96	0.64
3:J:470:LEU:HD13	3:J:471:SER:N	2.13	0.64
1:A:142:LEU:CD2	1:A:168:LEU:HD13	2.28	0.64
1:B:13:PHE:CE1	1:B:116:ARG:HD3	2.32	0.64
1:B:803:GLU:O	1:B:806:ARG:HB3	1.98	0.64
3:E:165:LEU:CD1	3:J:151:VAL:HG13	2.18	0.64
3:E:201:ARG:HG2	3:E:243:GLU:OE1	1.97	0.64
1:G:234:ARG:HH21	1:G:859:LEU:HA	1.63	0.64
1:B:56:LEU:HD12	1:B:60:LEU:HD23	1.80	0.64
1:B:269:TRP:CE3	1:B:822:ILE:HG21	2.33	0.64
1:B:1001:LEU:HD23	1:B:1018:ILE:HD12	1.79	0.64
2:C:194:LEU:HD21	2:C:213:LEU:CD2	2.27	0.64
2:D:42:THR:HG23	2:D:42:THR:O	1.96	0.64
1:F:877:LEU:O	1:F:877:LEU:HD12	1.97	0.64
1:G:39:THR:HG22	1:G:1047:VAL:HG12	1.79	0.64
2:H:107:ASP:OD2	2:I:43:ARG:HD3	1.97	0.64
3:J:98:ASP:OD1	3:J:98:ASP:O	2.14	0.64
3:J:375:LYS:HD3	3:J:376:GLU:H	1.63	0.64
1:A:887:GLN:HB2	1:A:890:ARG:HB2	1.80	0.64
1:B:223:GLU:OE1	1:B:223:GLU:N	2.31	0.64
1:B:893:ARG:HD3	1:B:967:MET:SD	2.38	0.64
2:D:230:ILE:O	2:D:234:THR:HG22	1.97	0.64
3:E:18:GLN:HE22	1:F:849:ASN:HB2	1.62	0.64
1:G:223:GLU:OE1	1:G:223:GLU:N	2.30	0.64
1:G:803:GLU:O	1:G:806:ARG:HB3	1.98	0.64
1:G:1001:LEU:HD23	1:G:1018:ILE:HD12	1.78	0.64
3:J:413:LEU:HD11	3:J:449:TRP:HE1	1.62	0.64
1:A:61:CYS:SG	1:A:206:ASN:HB2	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:O	1:A:909:LYS:HG3	1.97	0.64
1:A:1052:ASN:O	1:A:1055:MET:HE3	1.98	0.64
1:B:220:ILE:HD11	1:B:993:ALA:HB1	1.80	0.64
2:D:222:LEU:HD22	3:E:375:LYS:O	1.98	0.64
1:F:52:LEU:CD1	1:F:1077:MET:HE1	2.26	0.64
1:G:107:VAL:HG21	1:G:160:TYR:CE1	2.30	0.64
1:B:159:VAL:CG1	1:B:167:LEU:HG	2.27	0.64
2:C:158:ILE:HD11	2:C:204:ILE:CG2	2.27	0.64
1:G:181:TYR:HD2	1:G:187:TYR:HB2	1.63	0.64
3:J:243:GLU:O	3:J:243:GLU:HG2	1.98	0.64
1:A:1070:ARG:HH12	1:A:1073:GLN:HA	1.63	0.64
1:F:815:ALA:CB	1:F:824:VAL:HG21	2.28	0.64
1:G:71:THR:HG22	1:G:74:HIS:H	1.63	0.64
1:A:282:TRP:HZ3	1:A:782:GLU:HB2	1.62	0.63
2:C:55:LEU:CA	2:C:61:LEU:HD11	2.27	0.63
2:C:63:GLU:HB2	2:C:70:TYR:CE1	2.33	0.63
2:C:83:ILE:HG22	2:C:84:LEU:HD12	1.81	0.63
1:F:228:ASP:HA	1:F:957:ARG:HE	1.63	0.63
3:J:133:GLN:O	3:J:136:ILE:HG22	1.98	0.63
3:J:206:TRP:CZ3	3:J:306:ARG:HB2	2.33	0.63
1:A:877:LEU:HD12	1:A:877:LEU:O	1.98	0.63
1:G:789:GLU:HB2	1:G:792:ARG:NH2	2.13	0.63
3:J:111:ILE:O	3:J:115:GLU:HG3	1.98	0.63
1:B:203:THR:O	1:B:207:ARG:HG2	1.99	0.63
1:B:830:GLN:NE2	1:B:834:GLU:OE2	2.26	0.63
3:E:131:THR:O	3:E:135:GLU:HG2	1.97	0.63
1:F:1005:LEU:HD22	1:F:1015:PHE:HB3	1.80	0.63
1:G:899:VAL:HA	1:G:961:GLU:OE1	1.99	0.63
2:H:219:LEU:HD11	3:J:332:LEU:HD21	1.80	0.63
1:A:806:ARG:HG3	1:B:806:ARG:HH21	1.64	0.63
1:B:105:LYS:HE3	1:B:130:ASP:HA	1.79	0.63
1:G:235:ALA:O	1:G:238:VAL:HG12	1.97	0.63
1:G:239:ALA:HB1	1:G:939:ARG:HD3	1.81	0.63
1:G:246:THR:HG23	1:G:928:TYR:OH	1.98	0.63
1:G:1059:ARG:HG3	3:J:443:LEU:HD22	1.81	0.63
2:I:165:LEU:CD1	2:I:182:LEU:HD23	2.28	0.63
1:B:59:LEU:HG	1:B:110:ILE:HD12	1.80	0.63
1:B:247:GLU:HA	1:B:250:GLN:OE1	1.98	0.63
2:C:138:GLN:O	2:C:141:VAL:HG12	1.98	0.63
2:D:66:LYS:HE3	2:D:66:LYS:CA	2.23	0.63
1:G:1050:THR:HG22	1:G:1053:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:159:ASP:HA	2:I:162:LEU:HD12	1.78	0.63
1:A:65:ARG:H	1:A:206:ASN:HD21	1.47	0.63
3:E:58:SER:HB3	3:E:78:PHE:HA	1.81	0.63
1:A:849:ASN:HB2	3:J:18:GLN:HE22	1.63	0.63
1:A:890:ARG:HD3	1:A:975:ILE:HD11	1.80	0.63
1:B:123:LEU:HD21	1:B:191:LEU:HD21	1.80	0.63
2:H:75:SER:HB2	2:H:76:HIS:CE1	2.34	0.63
3:J:95:VAL:CG2	3:J:102:PHE:HB2	2.28	0.63
3:J:318:LYS:O	3:J:319:THR:OG1	2.09	0.63
1:A:1083:GLU:O	1:A:1086:GLU:HG2	1.99	0.63
1:B:71:THR:HG22	1:B:74:HIS:H	1.64	0.63
3:E:233:ASN:OD1	3:E:234:ASP:N	2.32	0.63
1:F:806:ARG:HG3	1:G:806:ARG:HH11	1.64	0.63
1:G:20:LEU:HD12	1:G:26:PHE:HD1	1.63	0.63
2:H:230:ILE:O	2:H:233:GLN:HG3	1.99	0.63
2:I:226:LEU:HD21	3:J:385:LEU:HD21	1.80	0.63
3:E:151:VAL:HA	3:J:165:LEU:CD1	2.28	0.63
1:F:279:LEU:HB2	1:F:786:VAL:CG1	2.24	0.63
1:G:195:PHE:CA	1:G:1014:LEU:HD23	2.26	0.63
1:B:891:TYR:CZ	1:B:967:MET:HB2	2.34	0.62
3:E:262:ALA:O	3:E:266:ARG:HG3	1.99	0.62
2:C:225:TRP:O	2:C:228:GLU:HG2	1.99	0.62
1:F:153:LEU:O	1:F:153:LEU:HD12	1.99	0.62
1:F:899:VAL:HG12	1:F:901:HIS:H	1.63	0.62
1:G:881:MET:HG3	1:G:995:TYR:HE1	1.64	0.62
3:J:259:GLU:O	3:J:262:ALA:HB3	1.99	0.62
3:E:131:THR:OG1	3:E:134:ARG:NH2	2.31	0.62
3:E:136:ILE:HD11	3:J:267:LEU:HD22	1.80	0.62
1:B:107:VAL:CG1	1:B:128:TRP:HB3	2.16	0.62
1:B:189:ALA:HA	1:B:192:ARG:NH1	2.14	0.62
1:G:13:PHE:CE1	1:G:116:ARG:HD3	2.35	0.62
1:G:121:VAL:HG21	1:G:194:PHE:CE1	2.34	0.62
1:G:189:ALA:HA	1:G:192:ARG:NH1	2.14	0.62
1:G:203:THR:O	1:G:207:ARG:HG2	1.99	0.62
1:G:881:MET:HE3	1:G:892:LEU:O	2.00	0.62
1:G:889:ASP:O	1:G:890:ARG:HD2	1.99	0.62
1:G:1031:VAL:O	1:G:1035:ILE:HD12	1.98	0.62
2:I:42:THR:HG23	2:I:42:THR:O	1.97	0.62
1:A:228:ASP:HA	1:A:957:ARG:HE	1.63	0.62
1:B:247:GLU:O	1:B:250:GLN:HG2	1.99	0.62
2:D:198:PRO:HD2	2:D:198:PRO:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:151:VAL:CG1	3:J:165:LEU:HD11	2.19	0.62
3:E:461:ILE:CG1	3:E:484:THR:HB	2.30	0.62
1:G:27:HIS:HD2	1:G:1074:ASN:HB3	1.63	0.62
2:I:169:LEU:O	3:J:388:SER:OG	2.18	0.62
1:B:931:LEU:O	1:B:935:VAL:HG23	2.00	0.62
3:E:263:MET:CE	3:J:133:GLN:HA	2.30	0.62
3:E:461:ILE:CD1	3:E:464:GLN:HB2	2.29	0.62
1:F:990:GLU:OE1	1:F:1026:ARG:HB2	1.99	0.62
1:G:219:GLU:HB3	1:G:223:GLU:OE2	1.98	0.62
2:H:55:LEU:HB2	2:H:61:LEU:CD1	2.30	0.62
2:H:137:ARG:HG3	3:J:332:LEU:HD11	1.82	0.62
3:J:375:LYS:HD3	3:J:376:GLU:N	2.14	0.62
1:A:966:VAL:CG1	1:A:976:GLU:HB3	2.30	0.62
2:I:63:GLU:HB2	2:I:70:TYR:CD1	2.34	0.62
3:J:236:ASP:OD2	3:J:306:ARG:NH1	2.32	0.62
3:J:241:THR:HA	3:J:245:ARG:CG	2.26	0.62
3:J:267:LEU:O	3:J:271:LEU:HD12	2.00	0.62
3:J:448:VAL:HG12	3:J:452:MET:HE2	1.81	0.62
1:B:891:TYR:HD2	1:B:969:ARG:HD3	1.64	0.62
1:B:899:VAL:HG13	1:B:904:LEU:CD1	2.29	0.62
3:E:8:ARG:NH2	3:J:39:THR:OG1	2.27	0.62
3:E:179:HIS:CE1	3:E:180:GLN:HG3	2.35	0.62
1:F:217:ILE:O	1:F:220:ILE:HG12	1.99	0.62
1:G:87:VAL:HG22	1:G:100:ILE:CG2	2.28	0.62
1:G:105:LYS:HE2	1:G:130:ASP:HA	1.82	0.62
2:H:83:ILE:O	2:H:86:PRO:HD2	2.00	0.62
3:J:83:ARG:O	3:J:87:GLU:HG2	2.00	0.62
1:A:834:GLU:OE1	3:J:241:THR:HB	2.00	0.62
1:B:30:HIS:HB3	1:B:1077:MET:HE2	1.80	0.62
1:B:53:VAL:O	1:B:57:MET:HG2	2.00	0.62
1:B:951:LYS:O	1:B:955:ASP:N	2.29	0.62
2:C:124:ARG:HB2	3:E:353:GLU:HG2	1.81	0.62
3:E:143:LEU:HD21	3:J:273:HIS:CD2	2.33	0.62
3:E:482:LEU:H	3:E:482:LEU:HD22	1.64	0.62
1:F:1056:ARG:HA	1:F:1059:ARG:HB2	1.81	0.62
1:A:57:MET:HE1	1:A:205:LEU:HD22	1.82	0.62
1:A:1024:PHE:CE1	1:A:1035:ILE:HG21	2.35	0.62
2:C:85:GLU:O	2:D:43:ARG:NH2	2.33	0.62
3:E:98:ASP:O	3:E:98:ASP:OD2	2.17	0.62
3:E:196:ARG:NH2	3:E:200:ARG:HD3	2.10	0.62
3:E:290:TRP:O	3:E:294:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD13	1:B:23:TRP:HB3	1.82	0.61
1:B:107:VAL:HG11	1:B:160:TYR:CE1	2.34	0.61
1:B:937:GLN:HA	1:B:940:ASP:OD2	1.99	0.61
3:E:198:ASP:HB3	3:E:243:GLU:OE2	2.00	0.61
3:E:469:GLU:OE1	3:E:477:ARG:HD3	2.01	0.61
1:G:878:ASN:HD21	1:G:893:ARG:HB2	1.64	0.61
3:J:314:ARG:HA	3:J:317:MET:CE	2.28	0.61
1:B:905:ARG:O	1:B:908:GLU:HG2	2.01	0.61
3:J:419:GLN:HG2	3:J:423:LYS:HE2	1.82	0.61
1:B:953:LEU:HD23	1:B:954:LEU:CD1	2.29	0.61
2:D:159:ASP:HA	2:D:162:LEU:HD12	1.82	0.61
1:G:1087:ARG:HG3	3:J:477:ARG:NH2	2.14	0.61
3:J:233:ASN:OD1	3:J:234:ASP:N	2.33	0.61
1:B:4:VAL:O	1:B:7:LEU:HG	2.00	0.61
3:E:260:LEU:HD12	3:E:292:VAL:HG13	1.82	0.61
1:F:974:VAL:HG21	1:F:977:SER:HB2	1.83	0.61
1:G:148:ASN:HB3	1:G:151:GLN:HG2	1.81	0.61
1:G:1084:GLU:HB2	3:J:478:TRP:CE3	2.36	0.61
1:A:57:MET:SD	1:A:206:ASN:HA	2.41	0.61
1:G:859:LEU:O	1:G:863:ILE:HG12	2.01	0.61
3:J:87:GLU:O	3:J:91:ARG:HB2	2.00	0.61
1:B:54:ASP:OD2	1:B:66:TYR:HB3	2.01	0.61
1:F:850:ARG:O	1:F:854:ASP:HB2	2.00	0.61
1:A:782:GLU:HG2	1:A:783:ILE:N	2.15	0.61
2:D:83:ILE:O	2:D:86:PRO:HD2	2.01	0.61
3:E:173:ILE:HD12	3:J:145:PRO:O	2.01	0.61
1:F:162:GLU:HG2	1:F:167:LEU:CD2	2.30	0.61
1:F:976:GLU:OE2	1:G:90:PRO:HD2	2.01	0.61
1:G:789:GLU:HA	1:G:792:ARG:HG2	1.81	0.61
2:I:230:ILE:O	2:I:234:THR:HG22	2.00	0.61
1:A:14:ILE:HD12	1:A:16:THR:HG22	1.83	0.61
1:A:976:GLU:OE2	1:B:90:PRO:HD2	2.00	0.61
1:B:51:THR:HG23	1:B:83:TYR:CE1	2.35	0.61
1:B:252:LEU:HD12	1:B:252:LEU:O	2.01	0.61
1:B:812:LEU:HD23	1:B:824:VAL:CG1	2.29	0.61
2:C:119:LEU:HD23	3:E:363:VAL:CG2	2.31	0.61
2:D:227:ARG:O	2:D:230:ILE:HG12	2.00	0.61
3:J:236:ASP:HB3	3:J:239:LEU:HG	1.82	0.61
1:A:983:GLY:N	1:B:77:ASP:OD2	2.32	0.61
1:B:242:PHE:HE2	1:B:932:GLN:HA	1.66	0.61
1:B:1050:THR:HG22	1:B:1053:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:SER:HB2	2:C:76:HIS:CE1	2.35	0.61
2:D:65:SER:OG	2:D:66:LYS:HD2	2.01	0.61
3:E:95:VAL:CG2	3:E:102:PHE:HB2	2.31	0.61
3:E:137:GLU:OE2	3:J:266:ARG:NH1	2.34	0.61
1:G:192:ARG:HD2	1:G:198:GLY:HA2	1.83	0.61
1:G:217:ILE:O	1:G:220:ILE:HB	2.01	0.61
1:A:128:TRP:CD1	1:A:160:TYR:HH	2.19	0.61
1:A:1036:ILE:HG21	1:A:1061:HIS:CB	2.31	0.61
1:B:105:LYS:HE2	1:B:130:ASP:HA	1.83	0.61
1:B:273:GLN:O	1:B:277:ARG:HG3	2.00	0.61
2:D:47:LYS:HA	2:D:47:LYS:HE2	1.83	0.61
2:D:103:LYS:HB2	3:E:370:GLU:OE2	2.01	0.61
3:E:243:GLU:OE1	3:J:122:MET:HE1	2.01	0.61
1:F:82:SER:HB2	1:F:87:VAL:HG22	1.83	0.61
1:F:832:LEU:HA	1:F:836:ALA:HB3	1.82	0.61
2:H:128:GLU:HG3	2:H:185:LEU:HD21	1.83	0.61
2:I:124:ARG:HA	3:J:373:ARG:O	2.01	0.61
1:B:890:ARG:HH21	1:B:975:ILE:HG12	1.66	0.60
3:E:472:ASP:OD2	3:E:478:TRP:NE1	2.33	0.60
2:H:223:LEU:HD21	3:J:334:GLU:HB3	1.83	0.60
3:J:165:LEU:HD12	3:J:165:LEU:O	2.00	0.60
3:J:242:PRO:HB2	3:J:243:GLU:OE1	2.01	0.60
2:C:223:LEU:HD21	3:E:334:GLU:HB3	1.81	0.60
3:E:158:ILE:HG23	3:J:158:ILE:HG12	1.83	0.60
3:E:414:ILE:O	3:E:418:LEU:HG	2.02	0.60
3:E:449:TRP:O	3:E:452:MET:HB2	2.01	0.60
1:A:991:ILE:HD12	1:A:1035:ILE:HD11	1.81	0.60
1:B:249:HIS:O	1:B:253:GLU:HG2	2.01	0.60
1:B:899:VAL:HA	1:B:961:GLU:OE1	2.00	0.60
2:D:165:LEU:HD12	2:D:182:LEU:HD23	1.84	0.60
3:E:192:ALA:HB1	3:E:291:LEU:CD1	2.31	0.60
1:G:130:ASP:OD2	1:G:140:LYS:HE3	2.01	0.60
2:I:131:LEU:O	2:I:135:ILE:HG13	2.00	0.60
1:A:1005:LEU:HD22	1:A:1015:PHE:HB3	1.83	0.60
3:E:266:ARG:HB3	3:J:140:GLU:OE1	2.01	0.60
1:F:64:PRO:HA	1:F:206:ASN:ND2	2.16	0.60
2:H:117:HIS:CE1	2:H:119:LEU:HB2	2.37	0.60
1:A:269:TRP:CD2	1:A:822:ILE:HG21	2.36	0.60
1:A:282:TRP:CZ3	1:A:782:GLU:HB2	2.36	0.60
1:B:940:ASP:HA	1:B:943:GLU:OE1	2.01	0.60
3:E:375:LYS:HD3	3:E:376:GLU:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1085:LEU:CD1	3:J:477:ARG:HH21	2.13	0.60
1:B:906:THR:O	1:B:909:LYS:HG2	2.01	0.60
1:F:14:ILE:HD12	1:F:16:THR:HG22	1.83	0.60
1:B:915:ASN:HA	1:B:918:ARG:CD	2.32	0.60
2:C:83:ILE:O	2:C:86:PRO:HD2	2.02	0.60
3:E:24:LEU:HD22	3:E:93:LEU:HD11	1.83	0.60
3:E:161:LEU:HD11	3:J:157:ARG:CB	2.30	0.60
3:E:265:GLU:O	3:E:268:ARG:HG2	2.02	0.60
1:G:1020:LEU:HD12	1:G:1023:ALA:HA	1.84	0.60
1:A:968:ASP:OD2	1:A:975:ILE:HG21	2.01	0.60
1:B:869:VAL:HA	1:B:872:GLU:HG2	1.84	0.60
2:C:164:GLN:HE21	1:F:919:PHE:CB	2.15	0.60
1:F:1056:ARG:NH2	3:J:406:ASN:HA	2.15	0.60
1:B:225:VAL:HG12	1:B:226:LEU:N	2.17	0.60
1:F:128:TRP:CD1	1:F:160:TYR:HH	2.19	0.60
1:F:893:ARG:HG2	1:F:894:LEU:N	2.17	0.60
3:J:179:HIS:CE1	3:J:180:GLN:HG3	2.37	0.60
1:B:915:ASN:HA	1:B:918:ARG:NE	2.17	0.60
1:G:40:ALA:HB1	1:G:1058:LEU:HD13	1.83	0.60
1:A:227:ASP:OD1	1:A:227:ASP:N	2.34	0.59
1:A:272:TYR:CA	1:A:793:LEU:HD23	2.31	0.59
1:F:221:PHE:CZ	1:F:894:LEU:HD21	2.36	0.59
1:G:1001:LEU:CD2	1:G:1018:ILE:HD12	2.32	0.59
1:B:191:LEU:HD13	1:B:195:PHE:HD1	1.67	0.59
2:D:124:ARG:HA	3:E:373:ARG:O	2.01	0.59
2:D:226:LEU:HD22	3:E:385:LEU:HD21	1.82	0.59
1:F:818:ASP:OD1	1:F:819:LEU:N	2.35	0.59
1:A:1024:PHE:CE2	1:A:1036:ILE:HD11	2.37	0.59
1:B:871:GLU:O	1:B:875:ASN:OD1	2.19	0.59
3:E:165:LEU:HD23	3:J:155:ARG:NE	2.16	0.59
2:I:143:TRP:HE1	2:I:151:ALA:HB1	1.68	0.59
1:A:796:GLU:O	1:A:800:ARG:HG2	2.02	0.59
1:B:218:ASP:O	1:B:222:ARG:HG3	2.02	0.59
1:B:235:ALA:O	1:B:238:VAL:HG12	2.01	0.59
1:B:242:PHE:O	1:B:242:PHE:HD1	1.85	0.59
3:E:472:ASP:CG	3:E:478:TRP:HE1	2.10	0.59
1:F:887:GLN:HB2	1:F:890:ARG:HB2	1.84	0.59
1:F:1024:PHE:CE2	1:F:1036:ILE:HD11	2.37	0.59
1:G:22:ASN:HB2	1:G:108:THR:HA	1.84	0.59
1:G:54:ASP:OD2	1:G:66:TYR:HB3	2.02	0.59
1:G:148:ASN:HB3	1:G:151:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:GLN:HE22	1:G:786:VAL:HB	1.67	0.59
1:B:130:ASP:OD2	1:B:140:LYS:HE3	2.02	0.59
1:B:253:GLU:CA	1:B:256:ARG:HE	2.05	0.59
1:B:801:MET:HE1	1:B:821:ASP:HB3	1.84	0.59
2:C:215:ASP:HB2	2:C:216:PRO:HD2	1.85	0.59
3:E:165:LEU:CD2	3:J:155:ARG:HG2	2.33	0.59
3:E:182:VAL:HG13	3:E:279:ALA:CB	2.33	0.59
1:F:12:SER:C	1:F:116:ARG:HD3	2.27	0.59
1:F:200:ASN:O	1:F:203:THR:HG22	2.02	0.59
1:F:221:PHE:HZ	1:F:894:LEU:HD21	1.67	0.59
1:G:271:LYS:HD2	1:G:271:LYS:O	2.02	0.59
2:C:143:TRP:CD2	2:C:154:ALA:HB2	2.36	0.59
3:E:57:LEU:O	3:E:61:LEU:HD23	2.01	0.59
1:G:895:ASP:OD2	1:G:963:ALA:HB3	2.02	0.59
2:H:69:LEU:O	2:H:73:VAL:HG23	2.02	0.59
2:H:124:ARG:HB3	3:J:353:GLU:OE1	2.02	0.59
2:H:158:ILE:HD11	2:H:204:ILE:HG21	1.84	0.59
3:J:122:MET:HB3	3:J:125:THR:HG23	1.84	0.59
1:A:818:ASP:OD1	1:A:819:LEU:N	2.35	0.59
1:B:1084:GLU:HB2	3:E:478:TRP:CE3	2.37	0.59
1:F:264:PRO:HB2	1:F:800:ARG:HD2	1.85	0.59
1:F:832:LEU:HD23	1:F:836:ALA:CB	2.33	0.59
1:F:968:ASP:OD2	1:F:975:ILE:HG21	2.03	0.59
3:J:62:ILE:O	3:J:65:VAL:HG22	2.02	0.59
3:J:108:GLU:CG	3:J:200:ARG:HG3	2.32	0.59
3:J:488:GLU:O	3:J:492:LEU:HG	2.03	0.59
1:B:40:ALA:CB	1:B:1058:LEU:HD13	2.33	0.59
1:B:51:THR:HG23	1:B:83:TYR:HE1	1.67	0.59
2:D:61:LEU:HD21	2:D:69:LEU:CB	2.32	0.59
2:D:124:ARG:NH2	3:E:373:ARG:HD3	2.18	0.59
2:D:172:PRO:CG	2:D:178:GLU:HG3	2.32	0.59
2:D:182:LEU:O	2:D:186:LEU:HG	2.03	0.59
3:E:236:ASP:HB3	3:E:239:LEU:HG	1.84	0.59
1:A:130:ASP:OD1	1:A:130:ASP:N	2.32	0.59
1:B:40:ALA:HB1	1:B:1058:LEU:HD13	1.85	0.59
1:F:37:ASP:HB2	1:F:1063:ARG:HG3	1.85	0.59
1:F:782:GLU:HG2	1:F:783:ILE:N	2.18	0.59
1:G:821:ASP:OD1	1:G:824:VAL:HB	2.03	0.59
1:A:96:GLY:H	1:A:99:HIS:CD2	2.21	0.59
1:A:128:TRP:CG	1:A:160:TYR:HH	2.21	0.59
3:E:267:LEU:HD22	3:J:136:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:VAL:HB	1:F:1049:ILE:HD13	1.85	0.59
1:F:96:GLY:H	1:F:99:HIS:CD2	2.21	0.59
1:F:227:ASP:N	1:F:227:ASP:OD1	2.33	0.59
1:G:120:GLN:HE22	1:G:122:ARG:CB	2.16	0.59
1:G:890:ARG:HH21	1:G:975:ILE:HG12	1.66	0.59
2:I:223:LEU:CD2	2:I:227:ARG:HH22	2.15	0.59
1:A:907:LEU:HD22	1:A:953:LEU:CD1	2.33	0.58
1:B:1020:LEU:HD12	1:B:1023:ALA:HA	1.85	0.58
2:D:107:ASP:O	2:D:109:THR:HG22	2.03	0.58
3:E:126:ALA:HB2	3:J:249:SER:OG	2.02	0.58
3:E:206:TRP:CZ3	3:E:306:ARG:HB2	2.38	0.58
1:F:990:GLU:OE2	1:F:1024:PHE:HA	2.03	0.58
1:F:1036:ILE:HG21	1:F:1061:HIS:CB	2.33	0.58
1:G:259:GLN:O	1:G:263:GLN:HG3	2.03	0.58
2:H:84:LEU:HB3	2:H:89:LEU:O	2.03	0.58
3:J:24:LEU:HD22	3:J:93:LEU:HD11	1.84	0.58
1:A:899:VAL:HG12	1:A:901:HIS:H	1.68	0.58
1:A:966:VAL:O	1:A:975:ILE:HG12	2.02	0.58
1:A:967:MET:HA	1:A:975:ILE:HG23	1.83	0.58
1:B:110:ILE:O	1:B:110:ILE:HG13	2.01	0.58
1:B:1017:THR:HA	1:B:1045:HIS:O	2.03	0.58
3:E:266:ARG:HH12	3:J:137:GLU:CD	2.09	0.58
3:J:263:MET:O	3:J:267:LEU:HD23	2.03	0.58
1:B:255:ALA:HB2	1:B:840:LYS:HZ2	1.67	0.58
1:B:805:LYS:HA	1:B:808:ASP:OD2	2.04	0.58
2:C:94:ASP:HB2	2:C:212:HIS:CE1	2.37	0.58
3:E:192:ALA:HB1	3:E:291:LEU:HD11	1.84	0.58
3:E:241:THR:HB	1:F:834:GLU:OE2	2.01	0.58
1:F:832:LEU:HD23	1:F:836:ALA:HB3	1.84	0.58
1:F:1039:LEU:HD21	1:F:1046:ALA:HB2	1.85	0.58
1:G:59:LEU:O	1:G:187:TYR:OH	2.20	0.58
1:G:940:ASP:HA	1:G:943:GLU:OE1	2.02	0.58
2:H:143:TRP:CD2	2:H:154:ALA:HB2	2.37	0.58
2:I:65:SER:OG	2:I:66:LYS:HD2	2.03	0.58
1:A:783:ILE:O	1:A:787:LYS:HG2	2.02	0.58
1:A:1020:LEU:HD12	1:A:1048:PHE:CE1	2.38	0.58
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.67	0.58
1:B:242:PHE:O	1:B:242:PHE:CD1	2.56	0.58
3:E:447:ALA:CA	3:E:450:ILE:HD12	2.26	0.58
1:F:81:ILE:CD1	1:F:139:MET:HE2	2.31	0.58
1:G:79:ASP:OD2	1:G:79:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:880:THR:HA	1:G:883:ARG:HG3	1.84	0.58
3:J:74:GLN:O	3:J:74:GLN:NE2	2.30	0.58
1:A:15:LEU:HD12	1:A:113:THR:O	2.03	0.58
1:A:196:GLU:OE1	2:C:177:LYS:NZ	2.32	0.58
1:A:907:LEU:HD22	1:A:953:LEU:HD11	1.85	0.58
1:B:153:LEU:O	1:B:157:LEU:HD23	2.03	0.58
1:B:1001:LEU:CD2	1:B:1018:ILE:HD12	2.33	0.58
3:E:310:GLU:O	3:E:313:VAL:HG12	2.03	0.58
1:F:269:TRP:CD2	1:F:822:ILE:HG21	2.38	0.58
1:F:782:GLU:HG2	1:F:783:ILE:H	1.67	0.58
2:H:94:ASP:HB2	2:H:212:HIS:CE1	2.38	0.58
3:J:420:LEU:CD2	3:J:437:LEU:HG	2.30	0.58
1:B:56:LEU:HD12	1:B:60:LEU:CD2	2.33	0.58
1:B:189:ALA:HA	1:B:192:ARG:HH12	1.67	0.58
2:D:165:LEU:CD1	2:D:182:LEU:HD23	2.33	0.58
3:E:133:GLN:O	3:E:136:ILE:HG22	2.04	0.58
3:E:144:ASN:HD21	3:E:150:ARG:HG3	1.67	0.58
1:F:282:TRP:HZ3	1:F:782:GLU:HB2	1.67	0.58
1:F:796:GLU:O	1:F:800:ARG:HG2	2.03	0.58
1:F:886:PHE:H	1:F:891:TYR:HA	1.68	0.58
2:H:124:ARG:HB2	3:J:353:GLU:HG2	1.85	0.58
3:E:271:LEU:HD21	3:E:285:ARG:O	2.03	0.58
1:F:192:ARG:NH1	1:F:199:GLU:HG3	2.19	0.58
1:F:806:ARG:HH22	1:G:806:ARG:HB2	1.68	0.58
1:F:897:LYS:HG2	1:F:898:LYS:N	2.19	0.58
1:F:987:GLY:HA3	1:G:45:THR:HG21	1.86	0.58
1:G:218:ASP:O	1:G:222:ARG:HG3	2.04	0.58
1:G:783:ILE:HD12	1:G:786:VAL:CG2	2.34	0.58
1:G:903:SER:O	1:G:906:THR:HG22	2.03	0.58
1:F:812:LEU:HD22	1:F:825:TYR:CD1	2.39	0.58
3:J:130:SER:HA	3:J:133:GLN:HG3	1.86	0.58
1:A:12:SER:C	1:A:116:ARG:HD3	2.28	0.58
1:A:176:ILE:HD12	2:C:187:ASP:OD2	2.04	0.58
1:B:50:THR:HG22	1:B:1021:ASP:OD2	2.04	0.58
1:B:168:LEU:O	1:B:171:MET:HG2	2.03	0.58
2:C:114:GLU:OE1	3:E:357:PRO:HA	2.04	0.58
1:G:116:ARG:HG2	1:G:116:ARG:HH11	1.68	0.58
1:G:145:PHE:HZ	1:G:194:PHE:CD1	2.22	0.58
1:G:849:ASN:HA	1:G:853:ASP:OD2	2.04	0.58
2:I:83:ILE:O	2:I:86:PRO:HD2	2.04	0.58
2:I:107:ASP:O	2:I:109:THR:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:24:LEU:HD22	3:J:93:LEU:CD1	2.34	0.58
3:J:182:VAL:HG13	3:J:279:ALA:HB2	1.84	0.58
1:A:224:LEU:HG	1:A:997:LEU:CD1	2.34	0.58
1:A:808:ASP:OD1	1:A:809:THR:N	2.37	0.58
1:B:87:VAL:HG22	1:B:100:ILE:CG2	2.27	0.58
1:B:217:ILE:HA	1:B:220:ILE:HB	1.85	0.58
1:B:248:ILE:HD13	1:B:847:TYR:CD2	2.37	0.58
2:C:158:ILE:HD11	2:C:204:ILE:HG21	1.86	0.58
3:E:24:LEU:HD22	3:E:93:LEU:CD1	2.33	0.58
3:E:461:ILE:HG13	3:E:484:THR:HB	1.86	0.58
3:E:465:ARG:HD3	3:E:481:ASN:ND2	2.18	0.58
1:G:891:TYR:CD2	1:G:969:ARG:HD3	2.37	0.58
1:G:899:VAL:HG13	1:G:904:LEU:CD1	2.34	0.58
3:J:402:TRP:O	3:J:405:PHE:HB3	2.04	0.58
1:A:851:SER:O	1:A:852:SER:HB3	2.03	0.57
1:B:242:PHE:HZ	1:B:932:GLN:HG3	1.69	0.57
3:E:161:LEU:HD22	3:J:158:ILE:CD1	2.34	0.57
1:F:282:TRP:CZ3	1:F:782:GLU:HB2	2.38	0.57
1:F:834:GLU:O	1:F:838:PRO:HG2	2.04	0.57
1:B:1019:ILE:HG23	1:B:1047:VAL:CG2	2.35	0.57
3:E:182:VAL:HG13	3:E:279:ALA:HB2	1.85	0.57
1:G:214:LEU:CD2	1:G:990:GLU:HG3	2.34	0.57
3:J:24:LEU:HD21	3:J:34:LEU:CD2	2.35	0.57
1:B:192:ARG:HD2	1:B:198:GLY:HA2	1.86	0.57
3:E:87:GLU:O	3:E:91:ARG:HB2	2.04	0.57
3:E:151:VAL:CG1	3:J:165:LEU:HD21	2.34	0.57
1:G:27:HIS:HA	1:G:102:ARG:HH22	1.69	0.57
1:G:834:GLU:O	1:G:838:PRO:HG2	2.04	0.57
1:G:916:ALA:HA	1:G:919:PHE:CE1	2.39	0.57
3:J:8:ARG:HA	3:J:11:ASN:OD1	2.04	0.57
3:J:177:GLU:HB2	3:J:180:GLN:HB2	1.85	0.57
1:G:68:LEU:HB3	1:G:210:GLY:HA3	1.86	0.57
1:G:832:LEU:HA	1:G:836:ALA:HB3	1.86	0.57
2:I:93:ILE:HD13	2:I:100:LEU:CD2	2.35	0.57
3:J:321:LEU:HA	3:J:324:GLU:OE1	2.05	0.57
1:B:214:LEU:CD2	1:B:990:GLU:HG3	2.35	0.57
1:B:976:GLU:HB3	1:B:978:ARG:O	2.04	0.57
2:C:69:LEU:H	2:C:69:LEU:HD12	1.68	0.57
1:F:810:GLY:O	1:F:813:VAL:N	2.31	0.57
1:G:23:TRP:HE3	1:G:108:THR:HG21	1.70	0.57
1:G:225:VAL:HG12	1:G:226:LEU:N	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:995:TYR:O	1:G:998:THR:OG1	2.19	0.57
1:G:1032:ALA:HA	1:G:1035:ILE:CD1	2.35	0.57
2:I:172:PRO:CG	2:I:178:GLU:HG3	2.34	0.57
3:J:210:ASP:O	3:J:214:ARG:HG3	2.03	0.57
1:A:62:ALA:HB2	1:A:188:LEU:CD1	2.34	0.57
1:B:252:LEU:HA	1:B:840:LYS:CE	2.33	0.57
1:B:1082:TRP:HB3	3:E:480:PHE:CD2	2.39	0.57
2:C:201:HIS:NE2	3:E:51:GLU:OE2	2.34	0.57
3:E:271:LEU:HD22	3:E:289:ARG:HB2	1.86	0.57
1:F:121:VAL:HG21	1:F:194:PHE:CE2	2.40	0.57
1:F:806:ARG:NH1	1:G:806:ARG:HA	2.14	0.57
2:H:66:LYS:HE3	2:H:69:LEU:CD1	2.34	0.57
2:H:114:GLU:OE1	3:J:357:PRO:HA	2.05	0.57
3:J:24:LEU:HB2	3:J:93:LEU:HD11	1.86	0.57
3:J:165:LEU:CD1	3:J:168:ALA:HB3	2.31	0.57
1:A:121:VAL:HG21	1:A:194:PHE:CZ	2.40	0.57
1:A:1057:LEU:O	1:A:1057:LEU:HD12	2.04	0.57
1:B:886:PHE:CE2	1:B:887:GLN:HG2	2.39	0.57
2:C:124:ARG:HB3	3:E:353:GLU:OE2	2.04	0.57
3:E:420:LEU:HD22	3:E:437:LEU:HG	1.85	0.57
1:F:815:ALA:HB2	1:F:824:VAL:HG21	1.87	0.57
2:H:54:GLU:HG3	2:H:69:LEU:CD2	2.34	0.57
2:I:124:ARG:CZ	3:J:373:ARG:HD3	2.35	0.57
3:E:162:GLU:HA	3:J:155:ARG:HH12	1.70	0.57
3:E:488:GLU:O	3:E:492:LEU:HG	2.05	0.57
1:F:207:ARG:NE	1:F:224:LEU:O	2.32	0.57
1:G:20:LEU:CD2	1:G:110:ILE:HG22	2.34	0.57
1:G:21:PHE:HD1	1:G:29:LEU:HA	1.68	0.57
2:I:114:GLU:N	2:I:114:GLU:OE1	2.38	0.57
1:B:151:GLN:HB3	1:B:156:TRP:HE1	1.70	0.57
1:B:899:VAL:HG22	1:B:901:HIS:H	1.68	0.57
1:G:27:HIS:CD2	1:G:1074:ASN:HB3	2.40	0.57
1:G:884:VAL:HG12	1:G:885:ASP:H	1.69	0.57
1:A:851:SER:O	1:A:931:LEU:HD21	2.04	0.57
1:A:1029:HIS:ND1	3:E:410:ARG:HD2	2.20	0.57
1:B:915:ASN:O	1:B:918:ARG:HD2	2.05	0.57
2:C:84:LEU:HB3	2:C:89:LEU:O	2.05	0.57
3:E:2:GLU:HG2	3:E:2:GLU:O	2.05	0.57
1:F:162:GLU:HG2	1:F:167:LEU:HD23	1.87	0.57
1:G:1017:THR:HA	1:G:1045:HIS:O	2.05	0.57
2:H:158:ILE:HD11	2:H:204:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:131:THR:O	3:J:135:GLU:HG2	2.05	0.57
1:A:58:THR:OG1	1:A:66:TYR:OH	2.17	0.56
1:A:1087:ARG:HB3	1:A:1091:ARG:NH2	2.19	0.56
1:B:263:GLN:HB2	1:B:264:PRO:HD3	1.87	0.56
1:B:989:LYS:HD2	1:B:989:LYS:O	2.04	0.56
2:D:70:TYR:CD1	2:D:100:LEU:HD11	2.39	0.56
1:F:32:ALA:CB	1:F:1077:MET:HE2	2.33	0.56
1:F:801:MET:HE2	1:F:822:ILE:HD11	1.88	0.56
1:F:887:GLN:OE1	1:F:888:PRO:HD2	2.05	0.56
2:H:143:TRP:CZ2	2:H:152:SER:HB3	2.36	0.56
3:J:260:LEU:HD12	3:J:292:VAL:HG13	1.86	0.56
1:B:127:LEU:CD1	1:B:139:MET:HE3	2.34	0.56
1:B:887:GLN:HB2	1:B:890:ARG:CG	2.34	0.56
2:D:122:ARG:NH1	3:E:373:ARG:HH21	2.03	0.56
2:D:126:ASN:HB2	2:D:129:GLN:OE1	2.05	0.56
3:E:120:ARG:HG2	3:J:201:ARG:NH2	2.19	0.56
3:E:139:LEU:HD22	3:J:188:VAL:HG21	1.87	0.56
3:E:263:MET:HE3	3:J:133:GLN:CD	2.29	0.56
1:F:851:SER:O	1:F:852:SER:HB3	2.05	0.56
1:G:975:ILE:HG22	1:G:976:GLU:OE1	2.06	0.56
3:J:157:ARG:O	3:J:161:LEU:HB2	2.04	0.56
3:J:408:LEU:HD23	3:J:408:LEU:C	2.30	0.56
1:B:62:ALA:HB2	1:B:188:LEU:HD13	1.88	0.56
1:B:845:LEU:HA	1:B:848:LEU:CG	2.33	0.56
1:B:859:LEU:O	1:B:863:ILE:HG12	2.04	0.56
2:D:209:ILE:HD11	3:E:369:ILE:CG2	2.36	0.56
1:F:968:ASP:HB2	1:F:971:SER:O	2.05	0.56
1:G:23:TRP:NE1	1:G:55:ALA:HB2	2.19	0.56
1:G:115:GLU:HA	1:G:115:GLU:OE2	2.05	0.56
1:G:121:VAL:HG21	1:G:194:PHE:CZ	2.41	0.56
1:G:126:LEU:HD11	1:G:157:LEU:CD1	2.35	0.56
1:G:144:LEU:HD12	1:G:156:TRP:CE3	2.40	0.56
1:G:199:GLU:OE2	1:G:200:ASN:N	2.39	0.56
1:G:1019:ILE:HG23	1:G:1047:VAL:CG2	2.35	0.56
2:H:194:LEU:HD21	2:H:213:LEU:CD2	2.35	0.56
2:I:124:ARG:NH2	3:J:373:ARG:HD3	2.21	0.56
2:I:227:ARG:NH1	2:I:227:ARG:HB2	2.19	0.56
2:C:156:ILE:CD1	2:C:161:LEU:HD11	2.35	0.56
2:D:121:ARG:O	3:E:371:ARG:HD2	2.06	0.56
3:E:18:GLN:NE2	1:F:849:ASN:HB2	2.20	0.56
1:G:812:LEU:HD23	1:G:824:VAL:CG1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:989:LYS:O	1:G:989:LYS:HD2	2.05	0.56
1:A:40:ALA:O	1:A:1065:ALA:HA	2.06	0.56
1:F:37:ASP:HB2	1:F:1063:ARG:CG	2.35	0.56
1:F:901:HIS:CD2	1:F:948:LEU:HG	2.41	0.56
1:G:142:LEU:CD1	1:G:144:LEU:HD21	2.31	0.56
1:G:142:LEU:CD2	1:G:180:THR:HG23	2.34	0.56
2:I:136:LEU:HD22	2:I:206:ILE:CD1	2.35	0.56
3:J:182:VAL:HG13	3:J:279:ALA:CB	2.34	0.56
3:J:271:LEU:CD2	3:J:289:ARG:HB2	2.35	0.56
1:A:228:ASP:HA	1:A:957:ARG:HH21	1.70	0.56
1:A:806:ARG:NH1	1:B:806:ARG:HA	2.20	0.56
1:B:812:LEU:CD2	1:B:825:TYR:HA	2.35	0.56
2:C:119:LEU:HD23	3:E:363:VAL:HG21	1.87	0.56
3:E:74:GLN:O	3:E:74:GLN:NE2	2.30	0.56
3:E:415:GLN:O	3:E:415:GLN:NE2	2.38	0.56
1:F:228:ASP:HA	1:F:957:ARG:HH21	1.71	0.56
1:F:1024:PHE:CE1	1:F:1035:ILE:HG21	2.41	0.56
2:I:122:ARG:NH1	3:J:373:ARG:HH21	2.04	0.56
3:J:477:ARG:HB3	3:J:477:ARG:CZ	2.34	0.56
1:A:272:TYR:HD1	1:A:793:LEU:HB3	1.71	0.56
1:A:991:ILE:HD12	1:A:1035:ILE:CD1	2.35	0.56
1:B:80:LEU:O	1:B:84:VAL:HG23	2.04	0.56
1:B:199:GLU:OE2	1:B:200:ASN:N	2.38	0.56
1:B:242:PHE:HD2	1:B:935:VAL:CB	2.18	0.56
1:B:261:SER:O	1:B:264:PRO:HD2	2.05	0.56
2:C:66:LYS:HE3	2:C:69:LEU:CD1	2.36	0.56
2:D:61:LEU:HD21	2:D:69:LEU:HB2	1.87	0.56
2:D:114:GLU:N	2:D:114:GLU:OE1	2.39	0.56
2:D:209:ILE:HD11	3:E:369:ILE:CB	2.35	0.56
3:E:40:LEU:HD11	3:E:53:ALA:HA	1.86	0.56
3:E:161:LEU:CD2	3:J:154:LEU:HD23	2.36	0.56
3:E:201:ARG:HG2	3:E:243:GLU:CD	2.30	0.56
1:F:142:LEU:O	1:F:144:LEU:HD12	2.06	0.56
1:G:220:ILE:O	1:G:224:LEU:HB3	2.06	0.56
3:J:265:GLU:HA	3:J:268:ARG:HD3	1.88	0.56
1:A:803:GLU:OE1	1:A:806:ARG:HD2	2.04	0.56
1:B:219:GLU:HB3	1:B:223:GLU:OE2	2.05	0.56
2:D:122:ARG:CZ	3:E:373:ARG:HH21	2.18	0.56
3:E:143:LEU:O	3:E:143:LEU:HD23	2.05	0.56
1:G:19:GLU:HB3	1:G:153:LEU:HD13	1.87	0.56
1:G:51:THR:HG23	1:G:83:TYR:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:886:PHE:CE2	1:G:887:GLN:HG2	2.40	0.56
1:G:887:GLN:HB2	1:G:890:ARG:CG	2.36	0.56
1:G:976:GLU:HB3	1:G:978:ARG:O	2.05	0.56
1:G:1020:LEU:HD12	1:G:1020:LEU:O	2.06	0.56
2:I:54:GLU:HA	2:I:54:GLU:OE2	2.06	0.56
3:J:86:ARG:O	3:J:90:LYS:HG2	2.06	0.56
1:A:893:ARG:HG2	1:A:894:LEU:H	1.71	0.56
1:B:40:ALA:O	1:B:1065:ALA:HA	2.06	0.56
1:B:172:GLU:HB2	1:B:180:THR:CG2	2.36	0.56
1:B:783:ILE:HD12	1:B:786:VAL:CG2	2.36	0.56
1:B:1020:LEU:HD12	1:B:1020:LEU:O	2.06	0.56
3:E:242:PRO:O	3:E:243:GLU:C	2.48	0.56
3:E:375:LYS:HD3	3:E:376:GLU:H	1.70	0.56
1:G:242:PHE:CE1	1:G:931:LEU:HB3	2.40	0.56
1:G:255:ALA:HB2	1:G:840:LYS:HZ2	1.70	0.56
3:J:70:TYR:HB2	3:J:72:ILE:HG13	1.87	0.56
1:B:145:PHE:HZ	1:B:194:PHE:CD1	2.24	0.56
1:G:249:HIS:O	1:G:253:GLU:HG2	2.06	0.56
1:G:255:ALA:HB2	1:G:840:LYS:HZ3	1.70	0.56
1:G:876:GLU:HA	1:G:879:GLU:OE1	2.06	0.56
2:H:133:VAL:HG22	2:H:194:LEU:HD23	1.87	0.56
1:A:52:LEU:HD11	1:A:1077:MET:HE1	1.88	0.55
1:A:92:ASP:C	1:B:981:SER:HB2	2.30	0.55
1:A:121:VAL:HG21	1:A:194:PHE:CE2	2.40	0.55
1:B:65:ARG:HG3	1:B:207:ARG:NH1	2.21	0.55
3:E:24:LEU:HD21	3:E:34:LEU:CD2	2.36	0.55
3:E:413:LEU:HD11	3:E:449:TRP:NE1	2.21	0.55
1:G:56:LEU:O	1:G:60:LEU:HD23	2.06	0.55
1:G:812:LEU:HD11	1:G:828:ARG:HG2	1.88	0.55
1:G:1054:GLU:HG2	1:G:1057:LEU:CG	2.36	0.55
3:J:239:LEU:HD22	3:J:245:ARG:HH21	1.70	0.55
1:A:66:TYR:O	1:A:76:SER:OG	2.15	0.55
1:B:199:GLU:OE2	1:B:199:GLU:N	2.39	0.55
3:E:408:LEU:HB2	3:E:441:HIS:CD2	2.41	0.55
3:E:415:GLN:O	3:E:418:LEU:HD12	2.06	0.55
1:G:244:GLY:C	1:G:248:ILE:HD12	2.31	0.55
1:G:252:LEU:HA	1:G:840:LYS:HZ3	1.71	0.55
3:J:130:SER:O	3:J:134:ARG:HG3	2.07	0.55
1:A:225:VAL:O	1:A:226:LEU:HD12	2.07	0.55
1:B:181:TYR:CD2	1:B:187:TYR:HA	2.41	0.55
1:B:887:GLN:HB2	1:B:890:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:MET:N	3:E:454:ARG:HH22	2.04	0.55
3:E:147:PRO:CG	3:J:173:ILE:HD13	2.36	0.55
3:E:495:ILE:HD11	3:E:497:TRP:CH2	2.41	0.55
1:F:1018:ILE:HD11	1:F:1039:LEU:HD11	1.89	0.55
1:G:252:LEU:HD12	1:G:252:LEU:O	2.06	0.55
2:H:201:HIS:NE2	3:J:51:GLU:OE2	2.35	0.55
2:I:126:ASN:HB2	2:I:129:GLN:OE1	2.05	0.55
1:A:61:CYS:O	1:A:184:LYS:NZ	2.30	0.55
1:F:92:ASP:HB2	1:G:980:GLY:O	2.05	0.55
1:G:12:SER:HB2	1:G:1014:LEU:HA	1.87	0.55
1:G:105:LYS:HG3	1:G:129:PHE:O	2.06	0.55
1:A:92:ASP:HB2	1:B:980:GLY:O	2.06	0.55
1:B:20:LEU:HD12	1:B:26:PHE:CD1	2.39	0.55
1:B:887:GLN:HB3	1:B:888:PRO:CD	2.35	0.55
3:E:24:LEU:O	3:E:27:THR:HG22	2.06	0.55
1:F:809:THR:O	1:F:809:THR:CG2	2.55	0.55
1:F:858:GLN:NE2	3:J:69:GLN:OE1	2.39	0.55
1:G:242:PHE:O	1:G:246:THR:N	2.26	0.55
2:H:60:LEU:HD12	2:H:60:LEU:O	2.05	0.55
1:A:192:ARG:NH1	1:A:199:GLU:HG3	2.22	0.55
1:B:945:ASN:OD1	1:B:946:ARG:HD3	2.07	0.55
2:D:78:GLU:O	2:D:81:THR:HG22	2.07	0.55
3:E:408:LEU:HD23	3:E:408:LEU:C	2.32	0.55
1:F:92:ASP:C	1:G:981:SER:HB2	2.31	0.55
1:G:151:GLN:HB3	1:G:156:TRP:HE1	1.72	0.55
1:G:270:GLU:HA	1:G:273:GLN:NE2	2.14	0.55
2:H:69:LEU:HD12	2:H:69:LEU:H	1.71	0.55
3:J:24:LEU:O	3:J:27:THR:HG22	2.05	0.55
3:J:143:LEU:O	3:J:143:LEU:HD23	2.07	0.55
3:J:257:SER:HA	3:J:261:LYS:HZ3	1.71	0.55
1:A:887:GLN:HB2	1:A:890:ARG:HG3	1.89	0.55
1:B:179:TRP:HB3	1:B:181:TYR:HE1	1.72	0.55
1:B:195:PHE:O	1:B:197:VAL:HG23	2.07	0.55
1:B:231:ALA:HB2	1:B:863:ILE:HD11	1.87	0.55
1:B:275:GLN:OE1	1:B:278:GLN:NE2	2.39	0.55
2:D:132:LEU:HD21	2:D:186:LEU:HD23	1.87	0.55
1:G:887:GLN:HB3	1:G:888:PRO:CD	2.34	0.55
1:G:953:LEU:HD23	1:G:954:LEU:CD1	2.36	0.55
2:H:136:LEU:HD23	2:H:161:LEU:HD21	1.88	0.55
1:A:41:VAL:HG12	1:A:49:LYS:HG2	1.87	0.55
1:B:951:LYS:HD3	1:B:958:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:GLU:HG2	1:B:1057:LEU:CG	2.36	0.55
3:E:223:HIS:O	3:E:227:ILE:HG12	2.07	0.55
1:F:887:GLN:HB2	1:F:890:ARG:CG	2.36	0.55
2:I:156:ILE:O	2:I:203:ARG:HG2	2.06	0.55
1:A:887:GLN:OE1	1:A:888:PRO:HD2	2.07	0.55
1:B:115:GLU:OE2	1:B:115:GLU:HA	2.05	0.55
1:B:975:ILE:HG22	1:B:976:GLU:OE1	2.05	0.55
3:E:54:ILE:CD1	3:E:82:SER:HA	2.37	0.55
3:E:70:TYR:HB2	3:E:72:ILE:HG13	1.88	0.55
1:F:808:ASP:CG	1:F:812:LEU:HB2	2.31	0.55
1:F:887:GLN:HB2	1:F:890:ARG:HG3	1.88	0.55
1:G:215:ASN:HB3	1:G:219:GLU:OE2	2.07	0.55
1:G:877:LEU:C	1:G:877:LEU:HD13	2.32	0.55
1:G:945:ASN:OD1	1:G:946:ARG:HD3	2.07	0.55
1:A:224:LEU:CD2	1:A:997:LEU:HD13	2.37	0.55
1:B:805:LYS:HA	1:B:808:ASP:CG	2.32	0.55
1:B:891:TYR:CD2	1:B:969:ARG:HD3	2.41	0.55
2:C:107:ASP:OD1	2:D:43:ARG:NH1	2.27	0.55
2:I:222:LEU:HD22	3:J:375:LYS:O	2.07	0.55
3:J:127:SER:O	3:J:128:ARG:HB3	2.06	0.55
1:B:242:PHE:HD2	1:B:935:VAL:HB	1.72	0.54
3:E:165:LEU:HD11	3:J:151:VAL:HA	1.87	0.54
1:F:242:PHE:O	1:F:246:THR:HG23	2.06	0.54
1:G:799:LYS:O	1:G:802:SER:OG	2.14	0.54
1:G:815:ALA:HB1	1:G:821:ASP:CG	2.31	0.54
1:G:899:VAL:HG22	1:G:901:HIS:H	1.72	0.54
2:H:47:LYS:HB2	2:H:47:LYS:NZ	2.22	0.54
1:A:267:LEU:HD22	1:A:271:LYS:NZ	2.22	0.54
1:B:280:ALA:HA	1:B:283:LEU:HB2	1.89	0.54
1:F:95:GLU:HG2	1:F:98:SER:H	1.73	0.54
1:F:196:GLU:OE1	2:H:177:LYS:NZ	2.36	0.54
1:F:253:GLU:HG3	1:F:254:THR:N	2.21	0.54
1:G:960:LEU:HD12	1:G:961:GLU:O	2.07	0.54
2:H:52:THR:HG21	2:H:83:ILE:HG21	1.89	0.54
2:H:136:LEU:CD2	2:H:161:LEU:HD21	2.37	0.54
2:I:226:LEU:HD23	3:J:385:LEU:HD21	1.89	0.54
1:A:95:GLU:HG2	1:A:98:SER:H	1.73	0.54
1:A:897:LYS:HG2	1:A:898:LYS:N	2.19	0.54
1:B:884:VAL:HG12	1:B:885:ASP:H	1.72	0.54
3:E:24:LEU:HB2	3:E:93:LEU:HD11	1.89	0.54
3:E:83:ARG:O	3:E:87:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:153:THR:HA	3:E:156:ARG:CZ	2.37	0.54
1:F:200:ASN:N	1:F:200:ASN:OD1	2.38	0.54
1:F:868:LEU:HD23	1:F:868:LEU:O	2.07	0.54
1:G:812:LEU:HD22	1:G:825:TYR:CD1	2.42	0.54
2:H:172:PRO:HG3	2:H:181:ARG:NH1	2.22	0.54
3:J:408:LEU:HB2	3:J:441:HIS:CD2	2.42	0.54
3:J:465:ARG:HD3	3:J:481:ASN:ND2	2.22	0.54
1:A:41:VAL:HB	1:A:1049:ILE:HD13	1.88	0.54
1:A:859:LEU:HD23	1:A:938:LEU:HD21	1.90	0.54
1:B:22:ASN:HA	1:B:102:ARG:NH1	2.23	0.54
1:B:253:GLU:HB3	1:B:256:ARG:HH21	1.72	0.54
3:E:418:LEU:HD12	3:E:419:GLN:H	1.70	0.54
1:F:864:GLU:OE1	1:F:864:GLU:HA	2.08	0.54
1:G:933:VAL:HG12	1:G:937:GLN:NE2	2.22	0.54
3:J:240:ASN:CG	3:J:242:PRO:HD2	2.32	0.54
1:A:887:GLN:HB2	1:A:890:ARG:CG	2.36	0.54
1:B:982:GLN:HG3	1:B:986:GLY:N	2.23	0.54
2:C:143:TRP:CZ2	2:C:152:SER:HB3	2.37	0.54
3:E:133:GLN:HA	3:J:263:MET:CE	2.34	0.54
3:E:243:GLU:CG	3:J:122:MET:HE1	2.38	0.54
3:E:378:ASP:OD1	3:E:380:GLU:N	2.41	0.54
1:F:1053:LYS:HB2	1:F:1054:GLU:OE2	2.07	0.54
1:G:251:GLU:O	1:G:840:LYS:NZ	2.40	0.54
3:J:92:ARG:HG3	3:J:92:ARG:NH1	2.22	0.54
3:J:114:VAL:HA	3:J:117:LEU:HD12	1.88	0.54
1:A:887:GLN:OE1	1:A:887:GLN:HA	2.07	0.54
1:B:23:TRP:HE3	1:B:108:THR:HG21	1.73	0.54
1:B:268:SER:HB3	1:B:797:LEU:CD2	2.38	0.54
2:D:136:LEU:HD22	2:D:206:ILE:CD1	2.37	0.54
1:F:803:GLU:OE1	1:F:806:ARG:HD2	2.08	0.54
1:F:1052:ASN:O	1:F:1055:MET:HE3	2.08	0.54
1:G:1032:ALA:HA	1:G:1035:ILE:HD13	1.90	0.54
2:I:60:LEU:HA	2:I:100:LEU:O	2.08	0.54
2:I:209:ILE:HD11	3:J:369:ILE:CB	2.37	0.54
3:J:84:GLU:HA	3:J:84:GLU:OE2	2.06	0.54
1:A:15:LEU:HD22	1:A:56:LEU:HD11	1.90	0.54
1:B:53:VAL:HG22	1:B:1019:ILE:HG21	1.90	0.54
3:E:413:LEU:O	3:E:417:THR:HG23	2.08	0.54
1:G:107:VAL:HG11	1:G:160:TYR:CE1	2.41	0.54
1:G:959:ARG:O	1:G:959:ARG:HG3	2.07	0.54
2:H:60:LEU:HD12	2:H:60:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:144:GLU:OE2	2:I:144:GLU:HA	2.08	0.54
3:J:1:MET:HG2	3:J:1:MET:O	2.08	0.54
1:A:886:PHE:H	1:A:891:TYR:HA	1.73	0.54
1:B:211:LEU:HD23	1:B:212:LYS:O	2.08	0.54
1:B:216:SER:HA	1:B:989:LYS:HE3	1.89	0.54
1:B:792:ARG:HB2	1:B:792:ARG:NH1	2.23	0.54
1:B:855:GLY:HA2	1:B:858:GLN:CG	2.38	0.54
1:B:1026:ARG:HD3	1:B:1026:ARG:N	2.23	0.54
1:B:1055:MET:HB2	3:E:444:GLU:OE2	2.08	0.54
2:C:62:GLU:OE1	2:C:208:PRO:HD2	2.07	0.54
3:E:423:LYS:HD3	3:E:423:LYS:N	2.22	0.54
1:G:828:ARG:NH1	1:G:832:LEU:HG	2.22	0.54
2:I:129:GLN:NE2	2:I:188:GLN:OE1	2.41	0.54
1:B:221:PHE:HB3	1:B:226:LEU:HD22	1.90	0.54
1:B:1032:ALA:HA	1:B:1035:ILE:HD13	1.90	0.54
3:E:267:LEU:O	3:E:271:LEU:HD12	2.08	0.54
1:G:890:ARG:NH2	1:G:975:ILE:HG12	2.22	0.54
1:G:937:GLN:HA	1:G:940:ASP:OD2	2.08	0.54
1:A:890:ARG:HG2	1:A:890:ARG:HH11	1.73	0.54
1:A:1070:ARG:NH1	1:A:1073:GLN:HA	2.23	0.54
1:B:144:LEU:HD22	1:B:156:TRP:CE3	2.43	0.54
1:B:216:SER:HA	1:B:989:LYS:CE	2.38	0.54
1:B:815:ALA:HB1	1:B:821:ASP:CG	2.33	0.54
1:B:959:ARG:O	1:B:959:ARG:HG3	2.08	0.54
1:B:1029:HIS:HB3	3:E:400:ASP:OD2	2.08	0.54
2:D:155:GLN:OE1	2:D:203:ARG:HD2	2.09	0.54
3:E:92:ARG:HG3	3:E:92:ARG:NH1	2.23	0.54
1:F:789:GLU:HA	1:F:789:GLU:OE2	2.07	0.54
1:F:892:LEU:CD2	1:F:964:VAL:HG13	2.35	0.54
1:A:810:GLY:O	1:A:813:VAL:N	2.31	0.53
1:A:901:HIS:CD2	1:A:948:LEU:HG	2.43	0.53
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.07	0.53
2:D:60:LEU:HD12	2:D:60:LEU:C	2.33	0.53
1:G:1026:ARG:HD3	1:G:1026:ARG:N	2.23	0.53
2:I:163:PRO:O	2:I:167:ILE:HG12	2.07	0.53
1:A:215:ASN:HB2	1:A:219:GLU:OE1	2.08	0.53
2:D:163:PRO:O	2:D:167:ILE:HG12	2.08	0.53
3:E:265:GLU:OE2	3:E:268:ARG:HD3	2.07	0.53
2:I:165:LEU:HD12	2:I:182:LEU:HD23	1.88	0.53
3:J:242:PRO:O	3:J:243:GLU:C	2.49	0.53
1:A:32:ALA:CB	1:A:1077:MET:HE2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ASP:HB2	1:A:971:SER:O	2.08	0.53
1:B:179:TRP:CD1	1:B:190:ARG:HH12	2.25	0.53
1:B:800:ARG:N	1:B:800:ARG:CD	2.72	0.53
3:E:128:ARG:O	3:E:128:ARG:HG3	2.07	0.53
3:E:195:LEU:HD11	3:J:132:VAL:HG11	1.90	0.53
1:F:56:LEU:HD23	1:F:56:LEU:O	2.08	0.53
1:F:66:TYR:O	1:F:76:SER:OG	2.18	0.53
1:F:252:LEU:HD21	1:F:256:ARG:NH2	2.23	0.53
1:F:274:LYS:HE2	1:F:277:ARG:HE	1.73	0.53
1:G:216:SER:HA	1:G:989:LYS:CE	2.39	0.53
1:G:269:TRP:CE3	1:G:822:ILE:HG21	2.44	0.53
1:G:799:LYS:HB2	1:G:799:LYS:NZ	2.24	0.53
1:G:897:LYS:HB3	1:G:961:GLU:OE2	2.08	0.53
1:G:1082:TRP:HB3	3:J:480:PHE:CD2	2.44	0.53
1:A:228:ASP:HA	1:A:957:ARG:NE	2.24	0.53
1:A:864:GLU:OE1	1:A:864:GLU:HA	2.07	0.53
2:C:117:HIS:CE1	2:C:119:LEU:HB2	2.43	0.53
2:D:197:SER:HB3	2:D:198:PRO:HD3	1.89	0.53
3:E:409:ASP:OD2	3:E:412:VAL:HB	2.09	0.53
1:F:887:GLN:OE1	1:F:887:GLN:HA	2.07	0.53
1:G:271:LYS:HG3	1:G:793:LEU:HD11	1.89	0.53
1:G:1029:HIS:C	1:G:1029:HIS:ND1	2.66	0.53
1:A:1053:LYS:HB2	1:A:1054:GLU:OE2	2.07	0.53
1:B:812:LEU:HD22	1:B:825:TYR:CD1	2.43	0.53
2:C:133:VAL:HG22	2:C:194:LEU:HD23	1.90	0.53
3:E:448:VAL:HG12	3:E:452:MET:HE2	1.89	0.53
1:F:228:ASP:HA	1:F:957:ARG:NE	2.23	0.53
1:G:65:ARG:HG3	1:G:207:ARG:NH1	2.22	0.53
2:H:107:ASP:OD1	2:I:43:ARG:NH1	2.28	0.53
3:J:233:ASN:CG	3:J:235:GLN:H	2.15	0.53
3:J:397:ILE:HD13	3:J:401:PHE:CD2	2.43	0.53
1:B:21:PHE:CE1	1:B:29:LEU:HB2	2.44	0.53
1:B:139:MET:HE3	1:B:141:ARG:HB3	1.89	0.53
1:B:890:ARG:NH2	1:B:975:ILE:HG12	2.22	0.53
2:C:54:GLU:HG3	2:C:69:LEU:CD2	2.39	0.53
2:D:124:ARG:CZ	3:E:373:ARG:HD3	2.39	0.53
3:E:108:GLU:HG2	3:E:200:ARG:HG3	1.89	0.53
1:G:262:LEU:CB	1:G:829:LEU:HD23	2.34	0.53
1:G:876:GLU:HA	1:G:879:GLU:CD	2.34	0.53
1:G:938:LEU:CD2	1:G:954:LEU:HD11	2.39	0.53
2:I:60:LEU:C	2:I:60:LEU:HD12	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PHE:HD1	1:B:29:LEU:HA	1.71	0.53
1:B:242:PHE:CD2	1:B:935:VAL:HB	2.44	0.53
1:B:247:GLU:HA	1:B:250:GLN:CD	2.34	0.53
1:B:953:LEU:C	1:B:954:LEU:HD12	2.33	0.53
3:E:257:SER:HA	3:E:261:LYS:HZ3	1.73	0.53
1:F:67:ASN:HD21	1:F:78:ARG:CZ	2.22	0.53
1:G:1077:MET:N	3:J:454:ARG:HH22	2.05	0.53
2:H:146:GLU:OE1	2:H:146:GLU:O	2.27	0.53
1:A:82:SER:HB2	1:A:87:VAL:HG22	1.91	0.53
3:E:267:LEU:HD11	3:E:288:LEU:HD11	1.90	0.53
1:G:7:LEU:O	1:G:11:GLU:HG2	2.09	0.53
1:G:43:GLY:O	1:G:49:LYS:NZ	2.41	0.53
1:G:126:LEU:C	1:G:127:LEU:HD22	2.34	0.53
1:G:887:GLN:HB2	1:G:890:ARG:HG2	1.90	0.53
1:G:982:GLN:HG3	1:G:986:GLY:N	2.23	0.53
1:G:1002:SER:OG	1:G:1042:PHE:HB3	2.09	0.53
2:I:215:ASP:CG	2:I:215:ASP:O	2.52	0.53
1:A:279:LEU:HD13	1:A:786:VAL:CG1	2.39	0.53
1:A:815:ALA:HB2	1:A:824:VAL:HG21	1.91	0.53
1:A:963:ALA:CB	1:A:979:THR:HA	2.39	0.53
2:C:117:HIS:O	2:C:120:VAL:HG12	2.09	0.53
3:E:255:ARG:HB3	3:E:255:ARG:NH1	2.24	0.53
1:F:82:SER:HB2	1:F:87:VAL:CG2	2.39	0.53
1:F:829:LEU:HD12	1:F:829:LEU:O	2.09	0.53
1:G:53:VAL:O	1:G:57:MET:HG2	2.09	0.53
1:G:252:LEU:HA	1:G:840:LYS:CE	2.39	0.53
1:G:905:ARG:O	1:G:908:GLU:HG2	2.08	0.53
1:G:1077:MET:O	3:J:454:ARG:NH2	2.41	0.53
2:I:73:VAL:HG11	2:I:100:LEU:HD13	1.89	0.53
3:J:108:GLU:HG2	3:J:200:ARG:HG3	1.88	0.53
1:A:53:VAL:HG22	1:A:1019:ILE:HG21	1.90	0.53
1:A:890:ARG:HD3	1:A:975:ILE:CD1	2.38	0.53
2:D:145:GLN:OE1	2:D:145:GLN:HA	2.09	0.53
3:E:138:ASN:ND2	3:J:134:ARG:HH11	2.06	0.53
1:F:1020:LEU:HD12	1:F:1048:PHE:CE1	2.44	0.53
1:G:40:ALA:CB	1:G:1058:LEU:HD13	2.37	0.53
1:G:906:THR:O	1:G:909:LYS:HG2	2.09	0.53
3:J:128:ARG:O	3:J:128:ARG:HG3	2.09	0.53
1:A:242:PHE:CZ	1:A:932:GLN:HA	2.44	0.52
1:B:1006:CYS:HA	1:B:1013:PRO:HA	1.92	0.52
1:F:225:VAL:O	1:F:226:LEU:HD12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:LEU:HD21	1:F:256:ARG:HH22	1.74	0.52
1:A:893:ARG:HG2	1:A:894:LEU:N	2.24	0.52
1:A:990:GLU:OE2	1:A:1024:PHE:HA	2.09	0.52
1:A:1031:VAL:HG12	1:A:1034:ARG:NH2	2.25	0.52
1:B:141:ARG:HH12	1:B:184:LYS:N	2.08	0.52
3:E:127:SER:O	3:E:128:ARG:HB3	2.08	0.52
3:J:378:ASP:C	3:J:378:ASP:OD1	2.52	0.52
1:A:960:LEU:HD23	1:A:960:LEU:H	1.75	0.52
1:B:855:GLY:HA2	1:B:858:GLN:HG2	1.92	0.52
2:D:143:TRP:HE1	2:D:151:ALA:HB1	1.72	0.52
3:E:135:GLU:HA	3:E:135:GLU:OE2	2.08	0.52
3:E:378:ASP:OD1	3:E:378:ASP:C	2.52	0.52
1:F:21:PHE:HA	1:F:28:GLY:O	2.09	0.52
1:F:265:VAL:HG23	1:F:800:ARG:HB3	1.90	0.52
1:F:801:MET:HE1	1:F:822:ILE:HG12	1.91	0.52
1:G:914:LEU:HD23	1:G:914:LEU:C	2.35	0.52
1:A:207:ARG:NE	1:A:224:LEU:O	2.33	0.52
1:B:262:LEU:HB3	1:B:829:LEU:HD23	1.90	0.52
1:B:1080:LEU:HD23	1:B:1080:LEU:C	2.35	0.52
1:F:61:CYS:SG	1:F:206:ASN:HB2	2.49	0.52
1:F:176:ILE:HD12	2:H:187:ASP:OD2	2.09	0.52
1:G:20:LEU:HD12	1:G:26:PHE:CD1	2.44	0.52
1:G:216:SER:HA	1:G:989:LYS:HE3	1.91	0.52
1:G:940:ASP:OD1	1:G:941:ALA:N	2.42	0.52
1:G:951:LYS:HD3	1:G:958:PHE:CE2	2.45	0.52
1:G:953:LEU:C	1:G:954:LEU:HD12	2.34	0.52
2:I:63:GLU:HB2	2:I:70:TYR:CE1	2.44	0.52
1:A:253:GLU:HG3	1:A:254:THR:N	2.25	0.52
1:B:35:HIS:HB2	1:B:1064:SER:HB3	1.91	0.52
1:B:901:HIS:HE1	1:B:903:SER:CB	2.22	0.52
3:E:162:GLU:HA	3:J:155:ARG:NH1	2.24	0.52
1:F:14:ILE:O	1:F:16:THR:HG23	2.08	0.52
1:F:789:GLU:OE1	1:F:792:ARG:NH2	2.36	0.52
1:G:117:GLU:HA	1:G:117:GLU:OE1	2.10	0.52
2:C:194:LEU:HD21	2:C:213:LEU:HD22	1.90	0.52
3:E:96:GLU:OE2	3:E:99:GLY:HA2	2.10	0.52
1:F:15:LEU:HD22	1:F:56:LEU:HD11	1.91	0.52
1:G:906:THR:HA	1:G:909:LYS:CD	2.39	0.52
2:H:144:GLU:O	2:H:147:SER:HB3	2.08	0.52
1:A:81:ILE:CD1	1:A:139:MET:HE2	2.39	0.52
1:A:832:LEU:HD23	1:A:836:ALA:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:PRO:HA	1:B:826:LEU:HD12	1.90	0.52
2:D:137:ARG:HD3	2:D:210:ILE:CG2	2.39	0.52
2:D:144:GLU:HA	2:D:144:GLU:OE2	2.10	0.52
3:E:165:LEU:HD12	3:E:165:LEU:O	2.10	0.52
1:F:890:ARG:HG2	1:F:890:ARG:HH11	1.75	0.52
1:G:1055:MET:HB2	3:J:444:GLU:OE2	2.09	0.52
2:H:45:LEU:CD1	2:H:48:ILE:HD12	2.28	0.52
3:J:423:LYS:HD3	3:J:423:LYS:N	2.23	0.52
3:J:466:GLU:OE1	3:J:466:GLU:N	2.43	0.52
1:A:37:ASP:HB2	1:A:1063:ARG:CG	2.40	0.52
2:C:46:GLN:HA	2:C:49:ARG:CZ	2.40	0.52
2:D:102:VAL:HG23	3:E:368:ALA:HA	1.91	0.52
1:F:230:SER:HA	1:F:956:PRO:HD3	1.92	0.52
1:G:275:GLN:OE1	1:G:278:GLN:NE2	2.42	0.52
1:G:787:LYS:O	1:G:787:LYS:HD3	2.10	0.52
1:G:1029:HIS:HB3	3:J:400:ASP:OD2	2.08	0.52
1:G:1071:ARG:HD2	3:J:455:GLU:O	2.10	0.52
2:I:109:THR:OG1	2:I:112:GLN:HB2	2.10	0.52
2:I:182:LEU:O	2:I:186:LEU:HG	2.10	0.52
1:A:21:PHE:HA	1:A:28:GLY:O	2.10	0.52
1:A:228:ASP:OD1	1:A:230:SER:N	2.28	0.52
2:C:85:GLU:HG2	2:D:43:ARG:NH2	2.24	0.52
1:F:242:PHE:CE1	1:F:931:LEU:HD23	2.44	0.52
1:F:983:GLY:N	1:G:77:ASP:OD1	2.41	0.52
1:G:126:LEU:HD11	1:G:157:LEU:HD11	1.91	0.52
1:G:179:TRP:CD1	1:G:190:ARG:HH12	2.28	0.52
1:G:855:GLY:HA2	1:G:858:GLN:NE2	2.22	0.52
1:G:925:GLU:N	1:G:925:GLU:OE2	2.42	0.52
2:H:54:GLU:HG3	2:H:69:LEU:HD22	1.92	0.52
2:H:117:HIS:HE1	2:H:119:LEU:HB2	1.75	0.52
2:H:175:GLU:OE1	2:H:179:ARG:NH2	2.42	0.52
3:J:24:LEU:HD21	3:J:34:LEU:HD21	1.90	0.52
3:J:62:ILE:HD11	3:J:77:PRO:CG	2.39	0.52
1:B:56:LEU:O	1:B:60:LEU:HD23	2.09	0.52
1:B:215:ASN:HB3	1:B:219:GLU:OE2	2.10	0.52
1:B:897:LYS:HB3	1:B:961:GLU:OE2	2.09	0.52
1:F:818:ASP:HB3	1:F:821:ASP:OD2	2.09	0.52
2:H:45:LEU:H	2:H:45:LEU:CD1	2.17	0.52
2:I:47:LYS:HA	2:I:47:LYS:CE	2.40	0.52
3:J:465:ARG:HD3	3:J:481:ASN:HD21	1.73	0.52
1:A:987:GLY:O	1:A:991:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:THR:HG21	1:A:1039:LEU:HA	1.91	0.51
1:B:914:LEU:HD23	1:B:914:LEU:C	2.35	0.51
3:E:397:ILE:HD13	3:E:401:PHE:CD2	2.45	0.51
2:H:215:ASP:HB2	2:H:216:PRO:HD2	1.92	0.51
3:J:495:ILE:HD11	3:J:497:TRP:CH2	2.46	0.51
1:A:142:LEU:HD11	1:A:180:THR:HB	1.92	0.51
2:C:144:GLU:O	2:C:147:SER:HB3	2.10	0.51
2:C:219:LEU:HD11	3:E:332:LEU:HD21	1.91	0.51
2:D:131:LEU:O	2:D:135:ILE:HG13	2.10	0.51
3:E:10:GLU:OE1	3:E:10:GLU:HA	2.10	0.51
1:F:29:LEU:HD21	1:F:154:GLU:HG2	1.93	0.51
1:F:875:ASN:C	1:F:875:ASN:OD1	2.52	0.51
1:G:263:GLN:HB2	1:G:264:PRO:HD3	1.91	0.51
3:J:57:LEU:O	3:J:61:LEU:HD23	2.10	0.51
1:A:225:VAL:HG23	1:A:226:LEU:HG	1.92	0.51
1:A:890:ARG:O	1:A:891:TYR:CD2	2.64	0.51
3:E:1:MET:O	3:E:1:MET:HG2	2.09	0.51
3:E:128:ARG:HB2	3:E:187:ASP:OD1	2.09	0.51
1:F:1070:ARG:NH2	4:F:1101:ADP:O4'	2.42	0.51
1:G:863:ILE:O	1:G:867:VAL:HG23	2.10	0.51
1:G:933:VAL:HG12	1:G:937:GLN:HE22	1.75	0.51
2:I:143:TRP:CE2	2:I:154:ALA:HA	2.45	0.51
3:J:261:LYS:H	3:J:261:LYS:CE	2.22	0.51
1:B:19:GLU:HB3	1:B:153:LEU:HD22	1.91	0.51
1:B:24:GLY:O	1:B:102:ARG:NH2	2.43	0.51
1:B:805:LYS:HA	1:B:808:ASP:OD1	2.10	0.51
2:C:128:GLU:HG2	3:E:350:ARG:O	2.10	0.51
3:E:233:ASN:CG	3:E:235:GLN:H	2.17	0.51
1:G:127:LEU:CD1	1:G:139:MET:HE3	2.41	0.51
1:G:160:TYR:HA	1:G:168:LEU:HD21	1.92	0.51
1:G:217:ILE:HD11	1:G:963:ALA:HA	1.92	0.51
1:G:1087:ARG:HG3	3:J:477:ARG:HH12	1.75	0.51
1:A:849:ASN:HB2	3:J:18:GLN:NE2	2.25	0.51
1:B:242:PHE:CZ	1:B:932:GLN:HA	2.45	0.51
1:B:909:LYS:HB2	1:B:912:ARG:HH22	1.75	0.51
3:E:482:LEU:HD22	3:E:482:LEU:N	2.26	0.51
1:F:960:LEU:HD23	1:F:960:LEU:H	1.75	0.51
1:G:146:SER:HB2	1:G:178:LEU:CD2	2.39	0.51
2:H:63:GLU:HB2	2:H:70:TYR:CE1	2.44	0.51
2:I:202:GLU:HA	2:I:202:GLU:OE1	2.10	0.51
1:A:809:THR:O	1:A:809:THR:CG2	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HG2	1:B:106:THR:HG21	1.92	0.51
1:B:116:ARG:NH1	1:B:117:GLU:HB3	2.23	0.51
1:B:819:LEU:HA	1:B:822:ILE:HG12	1.92	0.51
2:C:158:ILE:HD11	2:C:204:ILE:HG23	1.92	0.51
3:E:462:ASP:OD1	3:E:483:PRO:HB3	2.11	0.51
1:G:163:GLY:HA3	1:G:167:LEU:HB2	1.93	0.51
3:J:95:VAL:HG23	3:J:102:PHE:HB2	1.91	0.51
1:A:226:LEU:HD12	1:A:226:LEU:O	2.11	0.51
1:A:265:VAL:HG23	1:A:800:ARG:HB3	1.91	0.51
1:A:1021:ASP:OD1	1:A:1049:ILE:HB	2.11	0.51
1:B:142:LEU:HD13	1:B:142:LEU:C	2.36	0.51
2:D:143:TRP:O	2:D:146:GLU:HG3	2.10	0.51
2:D:202:GLU:OE1	2:D:202:GLU:HA	2.10	0.51
1:F:142:LEU:HD23	1:F:168:LEU:HD13	1.89	0.51
1:F:261:SER:O	1:F:264:PRO:HG2	2.09	0.51
1:F:878:ASN:OD1	1:F:894:LEU:HB2	2.11	0.51
1:F:890:ARG:HD3	1:F:975:ILE:HD11	1.93	0.51
1:G:1031:VAL:O	1:G:1034:ARG:N	2.42	0.51
1:B:148:ASN:HB3	1:B:151:GLN:HG3	1.93	0.51
3:E:431:ALA:H	3:E:466:GLU:CD	2.14	0.51
1:F:62:ALA:HB2	1:F:188:LEU:CD1	2.41	0.51
1:F:1057:LEU:HD12	1:F:1057:LEU:C	2.34	0.51
1:G:886:PHE:CD2	1:G:887:GLN:HG2	2.45	0.51
3:J:62:ILE:HA	3:J:65:VAL:HG13	1.91	0.51
1:A:224:LEU:HD21	1:A:997:LEU:HD13	1.92	0.51
1:A:858:GLN:NE2	3:E:69:GLN:OE1	2.44	0.51
1:B:204:LEU:HG	1:B:1001:LEU:HD13	1.92	0.51
1:B:253:GLU:OE1	1:B:256:ARG:CZ	2.58	0.51
3:E:124:SER:HB2	3:J:195:LEU:O	2.11	0.51
3:E:249:SER:OG	3:J:126:ALA:HB2	2.11	0.51
1:F:226:LEU:HD12	1:F:226:LEU:O	2.10	0.51
1:G:49:LYS:HB2	1:G:1049:ILE:CG2	2.41	0.51
1:G:894:LEU:HB3	1:G:964:VAL:HG22	1.92	0.51
1:G:1086:GLU:O	1:G:1087:ARG:C	2.54	0.51
3:J:227:ILE:HG23	3:J:228:VAL:N	2.26	0.51
3:J:257:SER:HA	3:J:261:LYS:HZ1	1.76	0.51
1:B:172:GLU:HB2	1:B:180:THR:HG23	1.93	0.51
1:B:796:GLU:CD	1:B:800:ARG:HD3	2.36	0.51
1:B:877:LEU:C	1:B:877:LEU:HD13	2.36	0.51
1:B:902:GLU:HA	1:B:905:ARG:NH1	2.26	0.51
1:G:199:GLU:OE2	1:G:199:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:55:LEU:CD1	2:I:61:LEU:HB2	2.41	0.51
2:D:65:SER:C	2:D:66:LYS:HD2	2.36	0.50
2:D:131:LEU:CD1	2:D:226:LEU:HD12	2.35	0.50
1:G:912:ARG:HB3	1:G:912:ARG:CZ	2.41	0.50
1:B:64:PRO:HG2	1:B:66:TYR:CZ	2.46	0.50
1:B:960:LEU:HD12	1:B:961:GLU:O	2.10	0.50
2:C:226:LEU:CD1	3:E:342:LEU:HD11	2.41	0.50
1:F:65:ARG:H	1:F:206:ASN:ND2	2.08	0.50
1:F:812:LEU:HD22	1:F:825:TYR:CE1	2.47	0.50
1:G:20:LEU:HD13	1:G:23:TRP:HB3	1.93	0.50
3:J:265:GLU:O	3:J:268:ARG:HG2	2.12	0.50
1:A:782:GLU:O	1:A:785:ARG:NH2	2.44	0.50
1:A:1070:ARG:NH1	1:A:1072:GLY:O	2.44	0.50
1:B:209:ALA:HA	1:B:1020:LEU:HA	1.93	0.50
1:B:881:MET:HE3	1:B:892:LEU:HG	1.93	0.50
1:B:886:PHE:CD2	1:B:887:GLN:HG2	2.46	0.50
2:D:109:THR:OG1	2:D:112:GLN:HB2	2.11	0.50
3:E:84:GLU:HA	3:E:84:GLU:OE2	2.11	0.50
3:E:134:ARG:NH1	3:J:138:ASN:HD22	2.07	0.50
3:E:169:GLU:OE2	3:J:151:VAL:HG11	2.10	0.50
1:F:215:ASN:HB2	1:F:219:GLU:OE1	2.11	0.50
1:F:250:GLN:CA	1:F:253:GLU:HG2	2.34	0.50
1:G:111:ALA:HB3	1:G:153:LEU:HD12	1.93	0.50
1:G:851:SER:O	1:G:852:SER:HB2	2.11	0.50
1:G:855:GLY:HA2	1:G:858:GLN:CG	2.42	0.50
3:J:34:LEU:HD13	3:J:114:VAL:HG21	1.93	0.50
3:J:146:ASN:OD1	3:J:148:ALA:N	2.44	0.50
1:A:65:ARG:H	1:A:206:ASN:ND2	2.09	0.50
1:A:985:SER:HB2	4:B:1101:ADP:O3A	2.12	0.50
1:A:1056:ARG:HH21	3:E:406:ASN:CA	2.18	0.50
3:E:125:THR:HB	3:E:183:GLU:OE2	2.12	0.50
3:E:176:LEU:HD21	3:J:142:ARG:NE	2.20	0.50
3:E:455:GLU:OE1	3:E:455:GLU:HA	2.11	0.50
2:H:70:TYR:HE2	2:H:100:LEU:HD21	1.76	0.50
2:H:124:ARG:HD3	3:J:353:GLU:HG3	1.93	0.50
3:J:288:LEU:HD12	3:J:288:LEU:O	2.12	0.50
3:J:413:LEU:HD12	3:J:417:THR:HG23	1.93	0.50
1:A:37:ASP:HB2	1:A:1063:ARG:HG3	1.94	0.50
1:A:247:GLU:HA	1:A:247:GLU:OE2	2.11	0.50
1:A:879:GLU:HG3	1:A:880:THR:N	2.27	0.50
1:B:21:PHE:O	1:B:108:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HG11	1:B:160:TYR:HE1	1.76	0.50
1:B:142:LEU:HD22	1:B:181:TYR:O	2.10	0.50
1:B:1050:THR:CG2	1:B:1053:LYS:H	2.24	0.50
1:B:1087:ARG:HA	1:B:1087:ARG:HE	1.76	0.50
2:D:49:ARG:O	2:D:52:THR:HG22	2.12	0.50
3:E:280:LEU:N	3:E:280:LEU:HD23	2.27	0.50
1:G:91:GLY:HA2	1:G:99:HIS:HB3	1.94	0.50
1:G:181:TYR:CD2	1:G:187:TYR:HB2	2.44	0.50
1:G:227:ASP:OD1	1:G:227:ASP:N	2.42	0.50
2:H:225:TRP:O	2:H:228:GLU:HG2	2.11	0.50
3:J:89:ILE:HD13	3:J:96:GLU:HB2	1.94	0.50
3:J:414:ILE:O	3:J:417:THR:OG1	2.25	0.50
1:A:122:ARG:CZ	1:A:122:ARG:HB2	2.42	0.50
1:B:916:ALA:HA	1:B:919:PHE:CE1	2.45	0.50
3:E:62:ILE:HA	3:E:65:VAL:CG1	2.42	0.50
3:E:165:LEU:HD23	3:J:155:ARG:HD3	1.91	0.50
1:F:142:LEU:HD11	1:F:180:THR:HB	1.93	0.50
1:G:836:ALA:O	1:G:840:LYS:HB3	2.11	0.50
2:H:62:GLU:OE2	2:H:208:PRO:HD2	2.11	0.50
2:H:96:ILE:HG21	3:J:321:LEU:HD11	1.94	0.50
3:J:290:TRP:O	3:J:294:ARG:HG2	2.12	0.50
1:B:79:ASP:OD2	1:B:79:ASP:N	2.45	0.50
1:B:234:ARG:HA	1:B:237:GLU:CD	2.36	0.50
1:B:912:ARG:HB3	1:B:912:ARG:CZ	2.42	0.50
3:E:50:LEU:O	3:E:54:ILE:HG12	2.12	0.50
3:E:178:THR:O	3:E:182:VAL:HG23	2.12	0.50
1:F:192:ARG:HH12	1:F:199:GLU:HG3	1.77	0.50
1:G:57:MET:HE3	1:G:206:ASN:HA	1.94	0.50
1:G:248:ILE:HD13	1:G:847:TYR:CD2	2.46	0.50
1:G:1080:LEU:HD23	1:G:1080:LEU:C	2.37	0.50
1:G:1085:LEU:HD12	3:J:477:ARG:HH21	1.77	0.50
3:J:241:THR:N	3:J:242:PRO:CD	2.75	0.50
1:A:818:ASP:HB3	1:A:821:ASP:OD2	2.11	0.50
1:B:23:TRP:NE1	1:B:55:ALA:HB2	2.26	0.50
1:B:242:PHE:CD2	1:B:935:VAL:HG21	2.47	0.50
1:B:278:GLN:NE2	1:B:786:VAL:HG12	2.27	0.50
1:B:278:GLN:HE21	1:B:786:VAL:HG12	1.77	0.50
3:E:129:LEU:HA	3:E:132:VAL:HG12	1.93	0.50
1:F:5:SER:HB3	1:F:37:ASP:OD2	2.11	0.50
1:G:144:LEU:HD12	1:G:156:TRP:CD2	2.47	0.50
1:G:253:GLU:OE1	1:G:256:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:137:ARG:HD3	2:I:210:ILE:CG2	2.41	0.50
1:B:181:TYR:HD2	1:B:187:TYR:CB	2.24	0.50
1:B:799:LYS:NZ	1:B:799:LYS:HB2	2.27	0.50
2:C:47:LYS:HZ3	2:C:47:LYS:HB2	1.76	0.50
1:G:64:PRO:HG2	1:G:66:TYR:CZ	2.47	0.50
1:G:139:MET:CE	1:G:141:ARG:HB3	2.42	0.50
1:G:217:ILE:HD11	1:G:963:ALA:CA	2.42	0.50
2:H:46:GLN:HA	2:H:49:ARG:CZ	2.42	0.50
2:I:196:THR:HG22	2:I:207:ARG:HD3	1.94	0.50
1:A:132:THR:O	1:A:132:THR:HG22	2.11	0.49
1:A:254:THR:O	1:A:258:GLN:HG3	2.12	0.49
1:A:274:LYS:CE	1:A:277:ARG:HE	2.24	0.49
1:B:906:THR:HA	1:B:909:LYS:CD	2.42	0.49
1:B:953:LEU:HD23	1:B:954:LEU:HD11	1.94	0.49
1:B:1086:GLU:O	1:B:1087:ARG:C	2.55	0.49
2:C:136:LEU:CD2	2:C:161:LEU:HD21	2.42	0.49
2:D:132:LEU:HD23	2:D:185:LEU:HB3	1.93	0.49
3:E:34:LEU:CD1	3:E:114:VAL:HG21	2.42	0.49
3:E:147:PRO:HG3	3:J:173:ILE:CD1	2.39	0.49
3:E:258:SER:HB2	3:E:259:GLU:OE2	2.11	0.49
1:G:876:GLU:O	1:G:879:GLU:HG2	2.12	0.49
1:G:915:ASN:HA	1:G:918:ARG:NE	2.27	0.49
2:I:155:GLN:OE1	2:I:203:ARG:HD2	2.12	0.49
3:J:158:ILE:O	3:J:162:GLU:N	2.34	0.49
1:A:275:GLN:OE1	1:A:275:GLN:HA	2.12	0.49
3:E:151:VAL:HG12	3:J:165:LEU:HD21	1.94	0.49
3:E:173:ILE:HD13	3:J:147:PRO:HG3	1.93	0.49
3:E:421:LEU:HD22	3:E:492:LEU:HD12	1.94	0.49
3:E:489:SER:O	3:E:493:MET:HG3	2.12	0.49
1:F:247:GLU:O	1:F:251:GLU:HG3	2.12	0.49
1:F:1021:ASP:OD1	1:F:1049:ILE:HB	2.12	0.49
1:F:1036:ILE:HD13	1:F:1036:ILE:N	2.26	0.49
1:G:113:THR:HB	1:G:120:GLN:HE21	1.77	0.49
3:J:105:ASP:O	3:J:109:VAL:HG23	2.11	0.49
1:A:195:PHE:O	1:A:197:VAL:HG13	2.12	0.49
1:B:879:GLU:O	1:B:883:ARG:HG3	2.11	0.49
1:B:955:ASP:OD2	1:B:957:ARG:NH2	2.42	0.49
2:D:187:ASP:C	2:D:187:ASP:OD1	2.55	0.49
2:D:226:LEU:HD22	3:E:385:LEU:CD2	2.43	0.49
1:F:963:ALA:HB1	1:F:979:THR:HA	1.93	0.49
1:G:822:ILE:HG22	1:G:826:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ASP:HB2	2:H:105:ARG:HB2	1.93	0.49
1:A:217:ILE:HG23	1:A:220:ILE:HD11	1.94	0.49
1:A:230:SER:HA	1:A:956:PRO:HD3	1.93	0.49
1:A:856:VAL:O	1:A:860:LEU:HG	2.12	0.49
1:B:792:ARG:NH1	1:B:792:ARG:CB	2.76	0.49
1:B:999:ALA:HB2	1:B:1042:PHE:HE1	1.76	0.49
1:B:1032:ALA:HA	1:B:1035:ILE:HD12	1.92	0.49
1:B:1070:ARG:HA	1:B:1075:SER:HA	1.95	0.49
1:G:27:HIS:HA	1:G:102:ARG:NH2	2.27	0.49
1:G:195:PHE:O	1:G:197:VAL:HG23	2.13	0.49
1:G:909:LYS:HB2	1:G:912:ARG:HH22	1.78	0.49
2:I:137:ARG:HD3	2:I:210:ILE:HG23	1.95	0.49
1:A:221:PHE:CE2	1:A:894:LEU:HD22	2.48	0.49
1:A:874:LEU:HD22	1:A:896:THR:HG22	1.95	0.49
1:A:1031:VAL:HG12	1:A:1034:ARG:HH21	1.77	0.49
1:B:192:ARG:HD2	1:B:198:GLY:C	2.38	0.49
1:B:883:ARG:HB3	1:B:883:ARG:CZ	2.42	0.49
1:B:901:HIS:CE1	1:B:903:SER:H	2.31	0.49
3:E:277:SER:HA	3:E:285:ARG:NH1	2.27	0.49
1:F:15:LEU:HD11	1:F:17:ARG:O	2.12	0.49
1:F:974:VAL:HG13	1:G:92:ASP:OD1	2.13	0.49
1:G:34:ILE:HG23	1:G:39:THR:CG2	2.43	0.49
1:G:107:VAL:HG22	1:G:128:TRP:HB2	1.92	0.49
1:G:822:ILE:N	1:G:823:PRO:HD2	2.26	0.49
1:G:881:MET:CE	1:G:893:ARG:HA	2.41	0.49
1:G:915:ASN:HA	1:G:918:ARG:CD	2.42	0.49
1:B:819:LEU:HD23	1:B:820:ASP:H	1.76	0.49
1:B:848:LEU:HD12	1:B:849:ASN:N	2.26	0.49
2:C:55:LEU:HA	2:C:61:LEU:CD1	2.37	0.49
1:F:269:TRP:CE3	1:F:822:ILE:HG13	2.48	0.49
1:F:1020:LEU:HB3	1:F:1023:ALA:HB2	1.93	0.49
2:H:47:LYS:HB2	2:H:47:LYS:HZ3	1.78	0.49
2:H:156:ILE:CD1	2:H:161:LEU:HD11	2.40	0.49
2:I:55:LEU:O	2:I:59:GLY:N	2.43	0.49
3:J:280:LEU:N	3:J:280:LEU:HD23	2.27	0.49
1:A:172:GLU:HB2	1:A:180:THR:HG21	1.94	0.49
1:B:30:HIS:HB3	1:B:1077:MET:CE	2.43	0.49
1:B:60:LEU:HD22	1:B:60:LEU:N	2.27	0.49
1:B:846:ASP:OD2	1:B:850:ARG:NH2	2.45	0.49
1:B:999:ALA:CB	1:B:1042:PHE:HE1	2.26	0.49
3:E:8:ARG:HA	3:E:11:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:ARG:CZ	3:E:163:ARG:HB2	2.43	0.49
3:E:257:SER:HA	3:E:261:LYS:HZ1	1.77	0.49
1:F:267:LEU:HD22	1:F:271:LYS:NZ	2.28	0.49
1:G:51:THR:HG23	1:G:83:TYR:CE1	2.48	0.49
1:G:148:ASN:CB	1:G:151:GLN:HE21	2.26	0.49
1:G:951:LYS:O	1:G:955:ASP:N	2.34	0.49
1:G:1018:ILE:HG23	1:G:1046:ALA:CB	2.43	0.49
2:I:187:ASP:C	2:I:187:ASP:OD1	2.55	0.49
3:J:421:LEU:HB3	3:J:489:SER:HB2	1.95	0.49
1:A:785:ARG:CZ	1:A:785:ARG:HB3	2.41	0.49
1:B:217:ILE:HD11	1:B:963:ALA:CA	2.42	0.49
1:B:227:ASP:OD1	1:B:227:ASP:N	2.42	0.49
1:B:864:GLU:HA	1:B:864:GLU:OE2	2.13	0.49
1:B:871:GLU:O	1:B:874:LEU:HB3	2.12	0.49
1:B:887:GLN:CB	1:B:888:PRO:HD2	2.37	0.49
2:D:63:GLU:HB2	2:D:70:TYR:CE2	2.48	0.49
3:E:89:ILE:HD13	3:E:96:GLU:HB2	1.93	0.49
1:F:132:THR:O	1:F:132:THR:HG22	2.12	0.49
1:F:856:VAL:O	1:F:860:LEU:HG	2.13	0.49
1:G:97:GLN:HB3	1:G:100:ILE:CD1	2.39	0.49
1:G:217:ILE:HD11	1:G:962:PHE:C	2.37	0.49
1:G:252:LEU:HD21	1:G:841:LEU:HD13	1.94	0.49
1:G:906:THR:HA	1:G:909:LYS:HG2	1.95	0.49
3:J:96:GLU:OE2	3:J:99:GLY:HA2	2.12	0.49
3:J:133:GLN:O	3:J:137:GLU:HG2	2.12	0.49
3:J:421:LEU:HD13	3:J:492:LEU:HD12	1.95	0.49
1:B:845:LEU:CA	1:B:848:LEU:HG	2.39	0.49
2:C:156:ILE:HG13	2:C:156:ILE:O	2.13	0.49
3:E:96:GLU:OE1	3:E:96:GLU:HA	2.13	0.49
3:E:217:ILE:HD13	3:E:317:MET:HG2	1.94	0.49
3:E:261:LYS:H	3:E:261:LYS:CE	2.23	0.49
1:F:142:LEU:HD22	1:F:168:LEU:HD13	1.93	0.49
1:G:20:LEU:CD1	1:G:26:PHE:HD1	2.25	0.49
1:G:796:GLU:OE1	1:G:797:LEU:HD22	2.13	0.49
1:G:974:VAL:HG21	1:G:977:SER:HA	1.93	0.49
2:H:158:ILE:HD12	2:H:186:LEU:HD11	1.95	0.49
3:J:413:LEU:HD12	3:J:413:LEU:O	2.13	0.49
3:J:437:LEU:O	3:J:439:PRO:HD3	2.13	0.49
1:B:252:LEU:HA	1:B:840:LYS:HE2	1.93	0.49
1:F:228:ASP:HA	1:F:957:ARG:NH2	2.28	0.49
1:F:952:ALA:O	1:F:959:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:LEU:HD13	2:H:48:ILE:CD1	2.30	0.49
1:A:228:ASP:HA	1:A:957:ARG:NH2	2.28	0.48
2:D:55:LEU:O	2:D:59:GLY:N	2.41	0.48
2:D:215:ASP:CG	2:D:215:ASP:O	2.56	0.48
3:E:242:PRO:HD3	1:F:834:GLU:HG3	1.93	0.48
3:J:40:LEU:HD11	3:J:53:ALA:HA	1.95	0.48
3:J:464:GLN:HB3	3:J:484:THR:OG1	2.13	0.48
1:A:5:SER:HB3	1:A:37:ASP:OD2	2.12	0.48
1:B:220:ILE:O	1:B:224:LEU:HB3	2.13	0.48
1:F:247:GLU:HA	1:F:247:GLU:OE2	2.13	0.48
1:G:153:LEU:HD23	1:G:153:LEU:C	2.38	0.48
2:I:65:SER:C	2:I:66:LYS:HD2	2.38	0.48
3:J:474:GLU:OE1	3:J:476:ARG:HB2	2.13	0.48
1:A:252:LEU:HD21	1:A:256:ARG:HH22	1.78	0.48
1:A:876:GLU:O	1:A:879:GLU:HG2	2.13	0.48
1:B:250:GLN:HA	1:B:253:GLU:HG2	1.95	0.48
1:B:1055:MET:HG3	3:E:444:GLU:HG3	1.95	0.48
2:D:60:LEU:HD12	2:D:60:LEU:O	2.13	0.48
1:F:985:SER:HB2	4:G:1101:ADP:O3A	2.13	0.48
1:G:71:THR:HG23	1:G:74:HIS:HB2	1.94	0.48
3:J:108:GLU:HG3	3:J:200:ARG:HG3	1.95	0.48
3:J:129:LEU:HA	3:J:132:VAL:HG12	1.95	0.48
3:J:135:GLU:OE2	3:J:135:GLU:HA	2.13	0.48
3:J:137:GLU:OE1	3:J:137:GLU:HA	2.13	0.48
3:J:178:THR:O	3:J:182:VAL:HG23	2.13	0.48
3:J:277:SER:HA	3:J:285:ARG:NH1	2.28	0.48
1:A:14:ILE:CD1	1:A:16:THR:HG22	2.43	0.48
1:B:191:LEU:HD21	1:B:195:PHE:HE1	1.78	0.48
3:E:24:LEU:HD21	3:E:34:LEU:HD21	1.95	0.48
2:I:207:ARG:HB2	2:I:209:ILE:HG22	1.95	0.48
1:A:123:LEU:HD22	1:A:191:LEU:HD21	1.95	0.48
1:A:247:GLU:O	1:A:251:GLU:HG3	2.13	0.48
1:A:952:ALA:O	1:A:959:ARG:HG3	2.13	0.48
1:B:252:LEU:HA	1:B:840:LYS:HZ3	1.78	0.48
3:E:151:VAL:HG13	3:J:165:LEU:HD21	1.96	0.48
1:F:17:ARG:HH11	1:F:17:ARG:HG3	1.78	0.48
1:F:82:SER:O	1:F:86:GLY:N	2.45	0.48
3:J:241:THR:OG1	3:J:245:ARG:NH1	2.45	0.48
1:B:91:GLY:HA2	1:B:99:HIS:HB3	1.94	0.48
1:B:788:ALA:O	1:B:791:HIS:HB3	2.13	0.48
1:B:881:MET:HG3	1:B:995:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:229:GLU:HG2	3:E:229:GLU:O	2.13	0.48
3:E:474:GLU:OE1	3:E:476:ARG:HB2	2.13	0.48
1:F:122:ARG:CZ	1:F:122:ARG:HB2	2.44	0.48
3:J:224:ARG:O	3:J:227:ILE:HG22	2.13	0.48
1:A:797:LEU:O	1:A:801:MET:HG3	2.13	0.48
1:A:1018:ILE:HD11	1:A:1039:LEU:HD11	1.95	0.48
1:A:1036:ILE:N	1:A:1036:ILE:HD13	2.28	0.48
1:B:251:GLU:O	1:B:840:LYS:NZ	2.46	0.48
2:C:143:TRP:CE3	2:C:154:ALA:HB2	2.49	0.48
2:D:225:TRP:CE3	2:D:226:LEU:HD23	2.48	0.48
3:E:173:ILE:HD13	3:J:147:PRO:CG	2.44	0.48
1:F:20:LEU:CD2	1:F:110:ILE:HG22	2.44	0.48
1:G:139:MET:HE3	1:G:141:ARG:HB3	1.96	0.48
1:G:883:ARG:CZ	1:G:883:ARG:HB3	2.43	0.48
1:G:1050:THR:CG2	1:G:1053:LYS:H	2.26	0.48
2:H:143:TRP:CE3	2:H:154:ALA:HB2	2.49	0.48
2:I:48:ILE:HD11	2:I:76:HIS:ND1	2.28	0.48
3:J:153:THR:HA	3:J:156:ARG:CD	2.42	0.48
3:J:263:MET:C	3:J:267:LEU:HD23	2.38	0.48
1:B:113:THR:HB	1:B:120:GLN:HE21	1.77	0.48
1:B:171:MET:O	1:B:175:ALA:N	2.43	0.48
2:C:62:GLU:HG3	2:C:99:LEU:HD12	1.95	0.48
1:G:933:VAL:O	1:G:937:GLN:NE2	2.45	0.48
1:G:983:GLY:N	1:G:988:GLU:H	2.10	0.48
1:G:1076:ASN:HB2	3:J:454:ARG:HH21	1.75	0.48
3:J:217:ILE:HD13	3:J:317:MET:HG2	1.95	0.48
3:J:248:ASP:OD1	3:J:306:ARG:NH2	2.47	0.48
3:J:414:ILE:HG22	3:J:418:LEU:HD11	1.94	0.48
1:A:991:ILE:CD1	1:A:1035:ILE:HD11	2.44	0.48
3:E:191:LEU:HD21	3:J:191:LEU:HD21	1.94	0.48
1:G:800:ARG:N	1:G:800:ARG:CD	2.76	0.48
3:J:144:ASN:HD21	3:J:150:ARG:HG3	1.78	0.48
1:A:27:HIS:O	3:E:387:LEU:HD11	2.13	0.48
1:B:822:ILE:N	1:B:823:PRO:HD2	2.29	0.48
2:C:96:ILE:HD12	3:E:319:THR:CB	2.44	0.48
3:E:266:ARG:O	3:E:270:ILE:HG13	2.14	0.48
1:F:1031:VAL:HG12	1:F:1034:ARG:NH2	2.29	0.48
1:G:1087:ARG:HE	1:G:1087:ARG:HA	1.79	0.48
2:I:109:THR:O	2:I:109:THR:HG23	2.14	0.48
3:J:472:ASP:CG	3:J:478:TRP:HE1	2.22	0.48
3:J:482:LEU:N	3:J:482:LEU:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PRO:HA	1:A:206:ASN:HD21	1.79	0.47
1:A:919:PHE:O	2:H:138:GLN:NE2	2.47	0.47
1:B:238:VAL:HG21	1:B:856:VAL:HG22	1.96	0.47
2:C:128:GLU:OE2	2:C:185:LEU:HD21	2.14	0.47
3:E:70:TYR:CB	3:E:72:ILE:HG13	2.44	0.47
3:E:152:ALA:HB3	3:E:156:ARG:HH21	1.79	0.47
3:E:290:TRP:HA	3:E:290:TRP:CE3	2.49	0.47
1:F:269:TRP:CE3	1:F:822:ILE:HG21	2.49	0.47
1:F:978:ARG:HA	1:G:90:PRO:HG3	1.96	0.47
1:G:141:ARG:HH12	1:G:184:LYS:N	2.07	0.47
1:G:1059:ARG:HB2	3:J:443:LEU:CD2	2.43	0.47
2:H:57:LYS:HE3	2:H:58:TYR:CZ	2.49	0.47
3:J:50:LEU:O	3:J:54:ILE:HG12	2.14	0.47
3:J:122:MET:HB3	3:J:125:THR:HG21	1.96	0.47
3:J:192:ALA:HB1	3:J:291:LEU:HD11	1.95	0.47
1:A:128:TRP:NE1	1:A:140:LYS:HB2	2.28	0.47
1:B:796:GLU:O	1:B:800:ARG:HD2	2.14	0.47
3:E:200:ARG:HD2	3:E:200:ARG:N	2.29	0.47
1:F:892:LEU:HD11	1:F:964:VAL:HG11	1.95	0.47
1:F:987:GLY:HA3	1:G:45:THR:CG2	2.43	0.47
2:H:106:LEU:O	2:H:106:LEU:HD12	2.14	0.47
2:I:91:ILE:O	2:I:91:ILE:HG13	2.14	0.47
1:A:16:THR:OG1	1:A:115:GLU:OE1	2.26	0.47
1:B:59:LEU:CD2	1:B:110:ILE:HD11	2.45	0.47
2:D:109:THR:O	2:D:109:THR:HG23	2.14	0.47
2:D:137:ARG:HD3	2:D:210:ILE:HG23	1.97	0.47
3:E:421:LEU:C	3:E:489:SER:HB2	2.39	0.47
1:F:998:THR:HG21	1:F:1039:LEU:HA	1.96	0.47
1:G:845:LEU:HD12	1:G:846:ASP:N	2.29	0.47
1:G:999:ALA:HB2	1:G:1042:PHE:HE1	1.78	0.47
1:G:1018:ILE:CG2	1:G:1046:ALA:HB2	2.44	0.47
2:I:60:LEU:HD12	2:I:60:LEU:O	2.14	0.47
2:I:222:LEU:HD12	3:J:377:VAL:HG12	1.96	0.47
1:A:272:TYR:HA	1:A:793:LEU:CD2	2.42	0.47
1:A:892:LEU:CD2	1:A:964:VAL:HG13	2.38	0.47
1:B:159:VAL:HG13	1:B:167:LEU:CG	2.42	0.47
1:B:851:SER:O	1:B:852:SER:HB2	2.13	0.47
2:C:96:ILE:HG21	3:E:321:LEU:HD11	1.95	0.47
3:E:146:ASN:OD1	3:E:148:ALA:N	2.45	0.47
3:E:267:LEU:HD12	3:E:288:LEU:HG	1.96	0.47
3:E:287:ASP:C	3:E:287:ASP:OD1	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:338:LEU:O	3:E:341:LYS:HG2	2.14	0.47
1:F:20:LEU:O	1:F:29:LEU:HD12	2.14	0.47
1:F:65:ARG:H	1:F:206:ASN:HD21	1.62	0.47
1:F:275:GLN:OE1	1:F:275:GLN:HA	2.13	0.47
1:G:113:THR:HG21	1:G:122:ARG:NH1	2.29	0.47
3:J:138:ASN:C	3:J:138:ASN:OD1	2.58	0.47
3:J:174:GLU:HA	3:J:174:GLU:OE1	2.14	0.47
1:A:1052:ASN:HA	1:A:1055:MET:CE	2.45	0.47
1:B:259:GLN:O	1:B:263:GLN:HG3	2.14	0.47
3:E:123:THR:OG1	3:J:194:SER:O	2.29	0.47
3:E:153:THR:HA	3:E:156:ARG:NH1	2.28	0.47
3:E:421:LEU:HD13	3:E:492:LEU:HD12	1.97	0.47
3:E:426:ARG:O	3:E:428:VAL:HG23	2.13	0.47
1:F:266:ALA:O	1:F:270:GLU:HG3	2.14	0.47
1:F:782:GLU:N	1:F:782:GLU:OE1	2.48	0.47
1:G:153:LEU:CD2	1:G:157:LEU:HD23	2.40	0.47
1:B:228:ASP:HA	1:B:957:ARG:NE	2.29	0.47
3:E:128:ARG:HA	3:E:131:THR:HB	1.96	0.47
3:E:152:ALA:CB	3:E:156:ARG:HH21	2.27	0.47
1:F:233:ASP:OD1	1:F:233:ASP:C	2.58	0.47
1:F:279:LEU:CD2	1:F:787:LYS:HE3	2.45	0.47
2:H:117:HIS:O	2:H:120:VAL:HG12	2.15	0.47
3:J:161:LEU:HD23	3:J:161:LEU:O	2.14	0.47
1:A:172:GLU:CG	1:A:180:THR:HG23	2.43	0.47
1:B:171:MET:HA	1:B:174:GLU:OE1	2.14	0.47
1:B:217:ILE:HD11	1:B:963:ALA:HA	1.97	0.47
1:B:239:ALA:HB1	1:B:939:ARG:CD	2.43	0.47
1:B:848:LEU:HD12	1:B:848:LEU:C	2.40	0.47
1:B:862:HIS:CE1	1:B:866:GLU:HG3	2.50	0.47
1:B:1018:ILE:HG23	1:B:1046:ALA:CB	2.44	0.47
2:D:78:GLU:HA	2:D:81:THR:HG22	1.96	0.47
2:D:106:LEU:HD23	2:D:106:LEU:HA	1.78	0.47
3:E:39:THR:HG21	3:J:5:THR:HG21	1.96	0.47
3:E:62:ILE:HD11	3:E:77:PRO:CG	2.44	0.47
3:E:86:ARG:O	3:E:90:LYS:HG2	2.15	0.47
3:E:105:ASP:O	3:E:109:VAL:HG23	2.14	0.47
3:E:487:LEU:CG	3:E:492:LEU:HD11	2.29	0.47
1:F:12:SER:HB3	1:F:1013:PRO:O	2.14	0.47
1:G:19:GLU:CB	1:G:153:LEU:HD13	2.45	0.47
1:G:30:HIS:CE1	1:G:1076:ASN:HB3	2.50	0.47
1:G:835:GLU:C	1:G:838:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:899:VAL:HG12	1:G:959:ARG:C	2.40	0.47
1:G:1059:ARG:HB2	3:J:443:LEU:HD22	1.96	0.47
2:H:199:ASP:C	2:H:199:ASP:OD1	2.57	0.47
2:I:209:ILE:HD11	3:J:369:ILE:HG12	1.97	0.47
3:J:70:TYR:CB	3:J:72:ILE:HG13	2.44	0.47
3:J:192:ALA:HB1	3:J:291:LEU:CD1	2.44	0.47
3:J:255:ARG:HB3	3:J:255:ARG:NH1	2.30	0.47
3:J:426:ARG:O	3:J:428:VAL:HG23	2.15	0.47
1:A:52:LEU:HD11	1:A:1077:MET:CE	2.45	0.47
1:A:966:VAL:HG13	1:A:976:GLU:HB3	1.97	0.47
1:A:1079:SER:O	2:D:177:LYS:NZ	2.44	0.47
1:B:151:GLN:OE1	1:B:178:LEU:HG	2.14	0.47
1:B:242:PHE:HD2	1:B:935:VAL:CG2	2.28	0.47
3:E:161:LEU:HD23	3:J:154:LEU:HD21	1.93	0.47
3:E:259:GLU:H	3:E:259:GLU:CD	2.22	0.47
1:F:782:GLU:O	1:F:785:ARG:NH2	2.47	0.47
1:G:812:LEU:CD2	1:G:825:TYR:HA	2.45	0.47
2:H:226:LEU:CD1	3:J:342:LEU:HD11	2.44	0.47
1:A:797:LEU:HD12	1:A:822:ILE:HD11	1.95	0.47
1:B:195:PHE:HA	1:B:1014:LEU:HD23	1.95	0.47
2:C:46:GLN:HA	2:C:49:ARG:NH2	2.30	0.47
2:C:155:GLN:HG2	2:C:205:VAL:HG22	1.96	0.47
2:C:199:ASP:C	2:C:199:ASP:OD1	2.58	0.47
2:D:61:LEU:HD21	2:D:69:LEU:HB3	1.95	0.47
3:E:173:ILE:CG2	3:J:147:PRO:HA	2.33	0.47
1:F:224:LEU:CD2	1:F:997:LEU:HD12	2.45	0.47
1:F:225:VAL:HG23	1:F:226:LEU:HG	1.97	0.47
1:G:163:GLY:O	1:G:166:ARG:HG2	2.14	0.47
2:H:96:ILE:HD12	3:J:319:THR:CB	2.42	0.47
2:I:227:ARG:O	2:I:230:ILE:HG12	2.15	0.47
3:J:271:LEU:HD21	3:J:285:ARG:O	2.15	0.47
3:J:287:ASP:C	3:J:287:ASP:OD1	2.58	0.47
1:B:7:LEU:O	1:B:11:GLU:HG2	2.15	0.47
1:B:64:PRO:HG2	1:B:66:TYR:OH	2.15	0.47
1:B:71:THR:HG23	1:B:74:HIS:HB2	1.97	0.47
1:B:120:GLN:HE22	1:B:122:ARG:CB	2.28	0.47
1:B:878:ASN:ND2	1:B:894:LEU:H	2.13	0.47
1:B:887:GLN:O	1:B:888:PRO:C	2.58	0.47
2:D:55:LEU:CD1	2:D:61:LEU:HB2	2.45	0.47
1:F:15:LEU:HD12	1:F:113:THR:O	2.14	0.47
1:F:185:LYS:CE	1:F:185:LYS:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:938:LEU:HD23	1:G:953:LEU:CD2	2.45	0.47
2:H:85:GLU:HG2	2:I:43:ARG:NH2	2.30	0.47
1:A:82:SER:HB2	1:A:87:VAL:CG2	2.45	0.46
1:A:887:GLN:HB2	1:A:890:ARG:CB	2.43	0.46
1:A:1029:HIS:CE1	3:E:410:ARG:HD2	2.50	0.46
1:A:1052:ASN:ND2	3:E:400:ASP:OD1	2.47	0.46
1:B:914:LEU:HD23	1:B:914:LEU:O	2.15	0.46
2:C:106:LEU:O	2:C:106:LEU:HD12	2.14	0.46
3:E:133:GLN:CD	3:J:263:MET:HE3	2.38	0.46
3:E:154:LEU:CA	3:J:161:LEU:HD21	2.45	0.46
3:E:437:LEU:O	3:E:439:PRO:HD3	2.14	0.46
1:F:195:PHE:O	1:F:197:VAL:HG13	2.15	0.46
1:F:228:ASP:OD1	1:F:230:SER:N	2.28	0.46
1:F:1040:ARG:HG2	1:F:1040:ARG:HH11	1.80	0.46
1:G:71:THR:HG22	1:G:74:HIS:N	2.30	0.46
1:G:902:GLU:HA	1:G:905:ARG:NH1	2.30	0.46
2:H:162:LEU:HB2	2:H:163:PRO:HD3	1.97	0.46
2:H:209:ILE:HD12	2:H:209:ILE:HA	1.82	0.46
2:I:122:ARG:CZ	3:J:373:ARG:HH21	2.27	0.46
3:J:290:TRP:HA	3:J:290:TRP:CE3	2.49	0.46
1:A:12:SER:HB3	1:A:1013:PRO:O	2.15	0.46
1:A:974:VAL:HG13	1:B:92:ASP:OD1	2.15	0.46
1:B:874:LEU:HD21	1:B:895:ASP:O	2.16	0.46
2:C:85:GLU:HG2	2:D:43:ARG:HH21	1.80	0.46
2:C:121:ARG:O	2:C:122:ARG:HB2	2.15	0.46
2:D:105:ARG:O	2:D:105:ARG:HG2	2.14	0.46
1:F:57:MET:SD	1:F:206:ASN:HA	2.55	0.46
1:G:272:TYR:HE1	1:G:790:LEU:CD2	2.26	0.46
1:G:955:ASP:OD2	1:G:957:ARG:NH2	2.45	0.46
1:G:1020:LEU:HD11	1:G:1048:PHE:HD1	1.80	0.46
1:A:806:ARG:HH22	1:B:806:ARG:CA	2.28	0.46
1:B:56:LEU:HD12	1:B:56:LEU:O	2.15	0.46
2:D:47:LYS:HA	2:D:47:LYS:CE	2.43	0.46
1:G:978:ARG:HH21	1:G:979:THR:HB	1.80	0.46
3:J:437:LEU:HD23	3:J:437:LEU:HA	1.76	0.46
1:A:17:ARG:HH11	1:A:17:ARG:HG3	1.79	0.46
1:A:252:LEU:HD21	1:A:256:ARG:NH2	2.30	0.46
1:B:192:ARG:HD2	1:B:198:GLY:CA	2.46	0.46
1:B:271:LYS:HD2	1:B:271:LYS:O	2.16	0.46
1:B:855:GLY:CA	1:B:858:GLN:HG2	2.46	0.46
2:C:172:PRO:HG3	2:C:181:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:174:GLU:HA	3:E:174:GLU:OE1	2.15	0.46
3:E:399:ASP:O	3:E:403:ASP:OD2	2.32	0.46
1:F:1055:MET:HE1	3:J:401:PHE:CD1	2.51	0.46
1:G:17:ARG:NH1	1:G:31:GLN:OE1	2.46	0.46
1:G:64:PRO:HG2	1:G:66:TYR:OH	2.15	0.46
1:G:228:ASP:HA	1:G:957:ARG:NE	2.30	0.46
1:G:1057:LEU:HD12	1:G:1058:LEU:H	1.80	0.46
2:H:46:GLN:C	2:H:46:GLN:OE1	2.59	0.46
1:A:15:LEU:HB3	1:A:1017:THR:HG21	1.98	0.46
1:A:41:VAL:HB	1:A:1049:ILE:CD1	2.45	0.46
1:B:17:ARG:NH1	1:B:31:GLN:OE1	2.47	0.46
1:B:783:ILE:HD12	1:B:786:VAL:HG23	1.97	0.46
1:B:989:LYS:HD2	1:B:989:LYS:C	2.40	0.46
3:E:135:GLU:OE1	3:J:135:GLU:OE1	2.33	0.46
1:F:783:ILE:O	1:F:787:LYS:HG2	2.15	0.46
1:F:981:SER:O	1:F:982:GLN:C	2.59	0.46
1:G:220:ILE:HD11	1:G:993:ALA:HB1	1.98	0.46
2:H:156:ILE:O	2:H:156:ILE:HG13	2.14	0.46
3:J:229:GLU:O	3:J:229:GLU:HG2	2.15	0.46
1:A:122:ARG:HB2	1:A:122:ARG:NH1	2.31	0.46
1:A:171:MET:HE2	1:A:171:MET:HB3	1.87	0.46
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.65	0.46
1:A:921:ASP:C	1:A:921:ASP:OD1	2.58	0.46
1:A:978:ARG:HA	1:B:90:PRO:HG3	1.97	0.46
1:B:978:ARG:HH21	1:B:979:THR:HB	1.81	0.46
1:B:1018:ILE:CG2	1:B:1046:ALA:HB2	2.46	0.46
1:B:1035:ILE:HD12	1:B:1035:ILE:H	1.81	0.46
1:B:1054:GLU:CD	1:B:1057:LEU:HD21	2.41	0.46
1:B:1057:LEU:HD12	1:B:1058:LEU:H	1.77	0.46
2:D:196:THR:HG22	2:D:207:ARG:HD3	1.96	0.46
3:E:95:VAL:HG23	3:E:102:PHE:HB2	1.96	0.46
2:I:93:ILE:HD13	2:I:100:LEU:HD21	1.98	0.46
2:I:105:ARG:O	2:I:105:ARG:HG2	2.15	0.46
3:J:265:GLU:HA	3:J:265:GLU:OE2	2.15	0.46
3:J:296:VAL:O	3:J:300:GLN:HG2	2.14	0.46
3:J:413:LEU:O	3:J:417:THR:HG23	2.16	0.46
3:J:424:GLU:HB3	3:J:426:ARG:HG2	1.97	0.46
1:A:87:VAL:HG12	1:A:100:ILE:HG13	1.96	0.46
1:A:90:PRO:HD2	4:A:1101:ADP:N3	2.30	0.46
1:A:1020:LEU:HB3	1:A:1023:ALA:HB2	1.97	0.46
1:B:179:TRP:HB3	1:B:181:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:LYS:O	1:B:787:LYS:HD3	2.16	0.46
1:B:842:ASN:HA	1:B:845:LEU:HD21	1.97	0.46
1:B:906:THR:HA	1:B:909:LYS:HG2	1.98	0.46
3:E:165:LEU:HD21	3:J:151:VAL:CG1	2.46	0.46
3:E:451:GLY:O	3:E:455:GLU:HB2	2.16	0.46
1:F:20:LEU:HD11	1:F:52:LEU:HD12	1.97	0.46
1:G:20:LEU:HD21	1:G:110:ILE:HG22	1.95	0.46
1:G:805:LYS:HA	1:G:808:ASP:CG	2.40	0.46
1:G:846:ASP:OD2	1:G:850:ARG:NH2	2.49	0.46
1:G:890:ARG:HH11	1:G:890:ARG:HG3	1.80	0.46
1:G:892:LEU:HD12	1:G:964:VAL:HG13	1.96	0.46
2:H:216:PRO:HD3	3:J:328:VAL:CG2	2.45	0.46
3:J:469:GLU:OE1	3:J:469:GLU:HA	2.16	0.46
1:B:105:LYS:HG3	1:B:129:PHE:O	2.16	0.46
1:B:115:GLU:OE1	1:B:120:GLN:HB2	2.16	0.46
1:B:983:GLY:N	1:B:988:GLU:H	2.12	0.46
2:C:126:ASN:HA	3:E:352:GLN:O	2.16	0.46
1:F:39:THR:HG21	1:F:1066:ILE:CD1	2.46	0.46
1:G:105:LYS:HE3	1:G:130:ASP:CA	2.45	0.46
1:G:889:ASP:O	1:G:889:ASP:OD1	2.34	0.46
1:G:944:ARG:HD3	1:G:944:ARG:N	2.31	0.46
2:H:121:ARG:O	2:H:122:ARG:HB2	2.15	0.46
3:J:128:ARG:HH21	3:J:191:LEU:HG	1.81	0.46
3:J:469:GLU:OE1	3:J:479:ARG:HA	2.16	0.46
1:B:876:GLU:HA	1:B:879:GLU:CD	2.40	0.46
1:B:881:MET:HE3	1:B:892:LEU:C	2.40	0.46
1:B:881:MET:CE	1:B:892:LEU:HG	2.45	0.46
1:B:894:LEU:H	1:B:894:LEU:HD23	1.81	0.46
2:D:143:TRP:CE2	2:D:154:ALA:HA	2.51	0.46
3:E:117:LEU:CD2	3:J:19:HIS:ND1	2.79	0.46
3:E:120:ARG:O	3:J:201:ARG:NH2	2.44	0.46
1:F:92:ASP:HB2	1:G:981:SER:HB2	1.96	0.46
1:F:907:LEU:HD22	1:F:953:LEU:HD11	1.97	0.46
1:F:1035:ILE:HG22	1:F:1036:ILE:HD13	1.98	0.46
1:G:122:ARG:HD2	1:G:151:GLN:O	2.16	0.46
3:J:472:ASP:OD2	3:J:478:TRP:NE1	2.46	0.46
1:B:42:ILE:HA	1:B:1050:THR:O	2.15	0.46
1:B:71:THR:HG22	1:B:74:HIS:N	2.30	0.46
1:B:97:GLN:HB3	1:B:100:ILE:CD1	2.38	0.46
1:B:120:GLN:HE22	1:B:122:ARG:HB2	1.81	0.46
1:B:142:LEU:CD1	1:B:144:LEU:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:LEU:HD12	1:B:846:ASP:N	2.31	0.46
1:B:890:ARG:HH11	1:B:890:ARG:HG3	1.80	0.46
3:E:210:ASP:O	3:E:214:ARG:HG3	2.15	0.46
3:E:231:LEU:HD23	3:E:231:LEU:HA	1.73	0.46
1:F:36:GLN:HG3	1:F:37:ASP:OD1	2.16	0.46
1:F:40:ALA:O	1:F:1065:ALA:HA	2.16	0.46
1:F:41:VAL:HB	1:F:1049:ILE:CD1	2.44	0.46
2:H:106:LEU:HB2	2:H:110:PRO:CG	2.45	0.46
3:J:38:LYS:O	3:J:38:LYS:HD2	2.16	0.46
1:A:92:ASP:HB2	1:B:981:SER:HB2	1.98	0.45
1:A:797:LEU:CD1	1:A:822:ILE:HD11	2.46	0.45
1:A:931:LEU:HD12	1:A:931:LEU:O	2.16	0.45
1:B:903:SER:HA	1:B:906:THR:HG22	1.97	0.45
2:C:54:GLU:HG3	2:C:69:LEU:HD22	1.97	0.45
2:C:90:ASP:HB2	2:C:105:ARG:HB2	1.98	0.45
3:E:155:ARG:CG	3:J:165:LEU:CD2	2.93	0.45
3:E:288:LEU:HD12	3:E:288:LEU:O	2.16	0.45
1:F:234:ARG:HD3	3:J:66:SER:HB2	1.98	0.45
1:G:30:HIS:HE1	1:G:1076:ASN:HB3	1.81	0.45
1:A:233:ASP:OD1	1:A:233:ASP:C	2.58	0.45
1:A:782:GLU:N	1:A:782:GLU:OE1	2.48	0.45
1:B:57:MET:HE2	1:B:206:ASN:HA	1.97	0.45
1:B:121:VAL:HG21	1:B:194:PHE:HE1	1.79	0.45
1:B:141:ARG:HH11	1:B:143:TRP:HZ2	1.63	0.45
1:B:899:VAL:HG12	1:B:959:ARG:C	2.41	0.45
2:C:46:GLN:C	2:C:46:GLN:OE1	2.59	0.45
3:E:6:ARG:O	3:E:10:GLU:HG2	2.16	0.45
3:E:491:ALA:O	3:E:495:ILE:HG23	2.15	0.45
1:F:221:PHE:O	1:F:226:LEU:HD11	2.16	0.45
1:F:806:ARG:HG3	1:G:806:ARG:NH1	2.29	0.45
1:G:88:SER:OG	1:G:1070:ARG:NH2	2.49	0.45
1:G:151:GLN:HG3	1:G:178:LEU:HD11	1.98	0.45
1:G:864:GLU:HA	1:G:864:GLU:OE2	2.15	0.45
3:J:409:ASP:OD2	3:J:412:VAL:HB	2.16	0.45
3:J:443:LEU:HA	3:J:446:PHE:HD2	1.82	0.45
1:A:14:ILE:O	1:A:16:THR:HG23	2.16	0.45
1:B:845:LEU:HA	1:B:848:LEU:CD2	2.46	0.45
1:B:1084:GLU:HB2	3:E:478:TRP:HZ3	1.79	0.45
2:D:121:ARG:HH22	2:D:123:GLN:CD	2.24	0.45
1:F:791:HIS:HA	1:G:791:HIS:HE1	1.82	0.45
1:G:894:LEU:HD23	1:G:894:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:999:ALA:HA	1:G:1042:PHE:CE1	2.52	0.45
2:I:165:LEU:HD11	2:I:182:LEU:HD23	1.97	0.45
1:A:53:VAL:O	1:A:57:MET:HG2	2.16	0.45
1:A:268:SER:OG	1:A:797:LEU:HD22	2.17	0.45
1:B:144:LEU:HD12	1:B:144:LEU:N	2.31	0.45
1:B:191:LEU:HD13	1:B:195:PHE:CD1	2.47	0.45
1:B:242:PHE:HD2	1:B:935:VAL:HG21	1.81	0.45
1:B:1019:ILE:HD13	1:B:1047:VAL:HG22	1.98	0.45
2:C:55:LEU:HD13	2:C:61:LEU:HD13	1.99	0.45
2:D:70:TYR:HD1	2:D:100:LEU:HD11	1.80	0.45
2:D:158:ILE:HG23	2:D:182:LEU:HD12	1.97	0.45
3:E:220:GLU:OE2	3:E:223:HIS:HA	2.17	0.45
3:E:421:LEU:HB3	3:E:489:SER:HB2	1.98	0.45
1:F:15:LEU:CD2	1:F:34:ILE:HD12	2.46	0.45
1:F:803:GLU:O	1:F:806:ARG:HB3	2.17	0.45
1:F:828:ARG:HA	1:F:828:ARG:HD2	1.85	0.45
1:F:890:ARG:O	1:F:891:TYR:CD2	2.69	0.45
1:G:238:VAL:HG22	1:G:856:VAL:HG22	1.99	0.45
1:G:253:GLU:HB3	1:G:256:ARG:HH21	1.81	0.45
1:G:1085:LEU:HB2	3:J:477:ARG:NH2	2.32	0.45
3:J:62:ILE:HD11	3:J:77:PRO:HG3	1.98	0.45
1:A:980:GLY:O	1:A:981:SER:C	2.59	0.45
1:B:126:LEU:O	1:B:127:LEU:HD22	2.17	0.45
1:B:876:GLU:HA	1:B:879:GLU:CG	2.47	0.45
2:C:41:GLU:OE2	2:C:42:THR:HG22	2.17	0.45
2:C:106:LEU:HB2	2:C:110:PRO:CG	2.46	0.45
3:E:23:ILE:HG22	3:E:88:TRP:CH2	2.51	0.45
3:E:194:SER:O	3:J:123:THR:HG22	2.17	0.45
1:F:1018:ILE:HD11	1:F:1039:LEU:CD1	2.47	0.45
1:F:1079:SER:O	2:I:177:LYS:NZ	2.46	0.45
1:G:272:TYR:CE1	1:G:790:LEU:HD21	2.47	0.45
1:G:901:HIS:ND1	1:G:903:SER:HB2	2.32	0.45
1:G:1080:LEU:HD23	1:G:1081:SER:N	2.32	0.45
1:G:1083:GLU:OE2	1:G:1085:LEU:HD23	2.17	0.45
1:A:801:MET:HE1	1:A:822:ILE:HG12	1.98	0.45
1:A:912:ARG:HH21	3:J:340:LEU:HD23	1.81	0.45
1:B:139:MET:CE	1:B:141:ARG:HB3	2.46	0.45
1:B:790:LEU:C	1:B:790:LEU:HD23	2.41	0.45
1:B:944:ARG:HD3	1:B:944:ARG:N	2.31	0.45
1:B:1028:SER:O	1:B:1031:VAL:HG22	2.16	0.45
2:D:141:VAL:O	2:D:145:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:155:ARG:HG2	3:J:165:LEU:HD23	1.99	0.45
3:E:189:TYR:CD1	3:E:189:TYR:C	2.94	0.45
3:E:253:GLN:HG3	3:J:126:ALA:HB1	1.98	0.45
3:E:368:ALA:O	3:E:370:GLU:N	2.49	0.45
1:G:42:ILE:HA	1:G:1050:THR:O	2.16	0.45
1:G:85:ARG:NE	1:G:134:SER:OG	2.50	0.45
1:G:855:GLY:O	1:G:857:THR:N	2.50	0.45
1:G:887:GLN:O	1:G:888:PRO:C	2.59	0.45
1:G:914:LEU:HD23	1:G:914:LEU:O	2.17	0.45
1:G:989:LYS:HD2	1:G:989:LYS:C	2.42	0.45
3:J:198:ASP:OD1	3:J:198:ASP:N	2.48	0.45
1:A:65:ARG:N	1:A:206:ASN:HD21	2.12	0.45
1:A:247:GLU:OE2	1:A:247:GLU:CA	2.64	0.45
1:B:145:PHE:CZ	1:B:194:PHE:CD1	3.04	0.45
1:B:997:LEU:HD12	1:B:1000:SER:OG	2.16	0.45
1:B:999:ALA:HA	1:B:1042:PHE:CE1	2.52	0.45
3:E:157:ARG:HB3	3:J:161:LEU:CD1	2.36	0.45
1:F:1054:GLU:HG2	1:F:1057:LEU:HD23	1.98	0.45
1:G:275:GLN:HE22	1:G:786:VAL:CB	2.29	0.45
1:G:796:GLU:O	1:G:800:ARG:HG2	2.16	0.45
1:G:803:GLU:OE1	1:G:803:GLU:N	2.50	0.45
3:J:54:ILE:CD1	3:J:82:SER:HA	2.46	0.45
1:B:71:THR:CG2	1:B:74:HIS:HB2	2.47	0.45
1:B:85:ARG:NE	1:B:134:SER:OG	2.49	0.45
1:B:829:LEU:C	1:B:829:LEU:HD13	2.42	0.45
2:D:158:ILE:HD12	2:D:202:GLU:HB3	1.99	0.45
3:E:173:ILE:HD13	3:J:147:PRO:CB	2.47	0.45
1:F:887:GLN:HB2	1:F:890:ARG:CB	2.46	0.45
1:G:116:ARG:HG2	1:G:116:ARG:NH1	2.32	0.45
1:G:252:LEU:HA	1:G:840:LYS:HE2	1.98	0.45
2:H:71:ARG:O	2:H:75:SER:OG	2.28	0.45
1:A:808:ASP:OD1	1:A:810:GLY:N	2.50	0.45
1:A:824:VAL:HG23	1:A:825:TYR:N	2.32	0.45
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.31	0.45
2:D:169:LEU:O	3:E:388:SER:OG	2.30	0.45
2:D:207:ARG:HB2	2:D:209:ILE:HG22	1.98	0.45
3:E:14:SER:HB3	1:F:850:ARG:NE	2.31	0.45
3:E:97:ARG:O	3:E:98:ASP:HB3	2.17	0.45
3:E:132:VAL:HG11	3:J:195:LEU:HD11	1.98	0.45
3:E:340:LEU:HD23	1:F:912:ARG:HH21	1.81	0.45
1:F:130:ASP:OD2	1:F:130:ASP:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:921:ASP:C	1:F:921:ASP:OD1	2.59	0.45
1:G:74:HIS:N	1:G:74:HIS:HD1	2.15	0.45
1:G:116:ARG:NH1	1:G:117:GLU:HB3	2.27	0.45
2:H:46:GLN:HA	2:H:49:ARG:NH2	2.31	0.45
1:A:23:TRP:NE1	1:A:55:ALA:HB2	2.33	0.45
1:A:874:LEU:CD2	1:A:896:THR:HG22	2.47	0.45
1:B:146:SER:OG	1:B:151:GLN:NE2	2.50	0.45
1:B:812:LEU:HD21	1:B:825:TYR:HA	1.99	0.45
2:C:47:LYS:HB2	2:C:47:LYS:NZ	2.31	0.45
3:E:138:ASN:ND2	3:J:134:ARG:NH1	2.66	0.45
1:F:234:ARG:HD3	3:J:66:SER:CB	2.47	0.45
1:F:985:SER:HB2	4:G:1101:ADP:PB	2.57	0.45
1:F:1056:ARG:HH21	3:J:406:ASN:CB	2.30	0.45
1:A:27:HIS:O	1:A:30:HIS:NE2	2.49	0.44
1:A:59:LEU:HD13	1:A:123:LEU:HB2	1.98	0.44
1:A:812:LEU:HG	1:A:825:TYR:CD1	2.52	0.44
1:A:1056:ARG:NH2	3:E:407:GLY:H	2.15	0.44
1:B:849:ASN:HA	1:B:853:ASP:OD2	2.17	0.44
1:B:1085:LEU:CD1	3:E:477:ARG:HD3	2.41	0.44
2:D:159:ASP:O	2:D:163:PRO:HD3	2.18	0.44
1:F:33:ALA:O	1:F:1066:ILE:HD11	2.16	0.44
1:F:34:ILE:HD13	1:F:1047:VAL:HG21	1.99	0.44
1:F:980:GLY:O	1:F:981:SER:C	2.60	0.44
1:G:874:LEU:HD21	1:G:894:LEU:CD1	2.48	0.44
1:G:1006:CYS:HA	1:G:1013:PRO:HA	1.99	0.44
3:J:378:ASP:OD1	3:J:380:GLU:N	2.50	0.44
3:J:440:ALA:O	3:J:441:HIS:ND1	2.48	0.44
1:A:81:ILE:CD1	1:A:129:PHE:HZ	2.30	0.44
1:B:258:GLN:OE1	1:B:808:ASP:HA	2.18	0.44
1:B:878:ASN:OD1	1:B:893:ARG:HB2	2.17	0.44
1:B:1042:PHE:O	1:B:1044:LEU:HD23	2.18	0.44
2:C:62:GLU:CG	2:C:99:LEU:HD12	2.47	0.44
3:E:154:LEU:CB	3:J:161:LEU:HD21	2.43	0.44
1:G:234:ARG:NH2	1:G:859:LEU:HA	2.30	0.44
1:G:999:ALA:CB	1:G:1042:PHE:HE1	2.30	0.44
3:J:128:ARG:HA	3:J:131:THR:HB	1.97	0.44
3:J:421:LEU:HD22	3:J:492:LEU:HD12	1.98	0.44
1:A:143:TRP:CE2	1:A:184:LYS:HG3	2.52	0.44
1:A:981:SER:O	1:A:982:GLN:C	2.59	0.44
1:B:20:LEU:CD1	1:B:26:PHE:HD1	2.29	0.44
1:B:271:LYS:CG	1:B:793:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:ILE:HD11	2:C:204:ILE:HD11	1.99	0.44
2:D:48:ILE:HD11	2:D:76:HIS:ND1	2.32	0.44
1:F:979:THR:HG23	1:F:979:THR:O	2.17	0.44
1:G:192:ARG:HD2	1:G:198:GLY:CA	2.47	0.44
3:J:432:GLU:OE1	3:J:432:GLU:N	2.44	0.44
1:A:54:ASP:OD2	1:A:83:TYR:OH	2.25	0.44
1:A:143:TRP:CH2	1:A:184:LYS:HE3	2.52	0.44
1:A:221:PHE:O	1:A:226:LEU:HD11	2.18	0.44
1:B:74:HIS:N	1:B:74:HIS:HD1	2.15	0.44
1:B:854:ASP:O	1:B:858:GLN:NE2	2.51	0.44
3:E:131:THR:HA	3:E:134:ARG:NE	2.27	0.44
1:F:1029:HIS:ND1	3:J:410:ARG:HD2	2.33	0.44
1:G:187:TYR:CZ	1:G:191:LEU:HD22	2.53	0.44
1:G:278:GLN:NE2	1:G:786:VAL:HG12	2.33	0.44
1:G:1055:MET:HG3	3:J:444:GLU:HG3	1.99	0.44
2:I:90:ASP:O	2:I:102:VAL:HA	2.17	0.44
2:I:162:LEU:HB2	2:I:163:PRO:HD3	2.00	0.44
3:J:291:LEU:O	3:J:294:ARG:HG3	2.18	0.44
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.67	0.44
1:B:68:LEU:HD12	1:B:68:LEU:HA	1.73	0.44
1:B:191:LEU:HD12	1:B:202:PHE:CE2	2.53	0.44
1:B:822:ILE:HG22	1:B:826:LEU:HD11	1.98	0.44
2:C:120:VAL:HG13	2:C:120:VAL:O	2.18	0.44
2:D:120:VAL:HG21	3:E:368:ALA:CB	2.48	0.44
1:F:143:TRP:CE2	1:F:184:LYS:HG3	2.53	0.44
1:F:274:LYS:CE	1:F:277:ARG:HE	2.29	0.44
1:G:142:LEU:HD13	1:G:142:LEU:C	2.42	0.44
1:G:167:LEU:O	1:G:171:MET:HG2	2.18	0.44
1:G:217:ILE:HA	1:G:220:ILE:HD12	1.99	0.44
1:G:867:VAL:HG13	1:G:960:LEU:HD23	1.99	0.44
1:G:874:LEU:HD21	1:G:894:LEU:HD11	2.00	0.44
3:J:50:LEU:HD21	3:J:86:ARG:CZ	2.48	0.44
1:A:1040:ARG:HG2	1:A:1040:ARG:HH11	1.83	0.44
1:B:974:VAL:HG21	1:B:977:SER:HA	1.99	0.44
1:B:1059:ARG:HB2	3:E:443:LEU:CD2	2.47	0.44
2:D:146:GLU:OE1	2:D:147:SER:OG	2.35	0.44
2:D:179:ARG:HG3	2:D:179:ARG:HH11	1.82	0.44
1:F:90:PRO:HD2	4:F:1101:ADP:N3	2.33	0.44
1:G:141:ARG:HH11	1:G:143:TRP:HZ2	1.65	0.44
1:G:837:LEU:HD23	1:G:837:LEU:HA	1.83	0.44
3:J:58:SER:HA	3:J:81:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:GLY:O	1:A:857:THR:N	2.51	0.44
1:B:799:LYS:HB3	1:B:800:ARG:HH11	1.81	0.44
3:E:61:LEU:HD12	3:E:72:ILE:HG23	2.00	0.44
3:E:103:ALA:CB	3:E:107:LEU:HD23	2.47	0.44
1:F:108:THR:HG22	1:F:127:LEU:O	2.17	0.44
1:F:122:ARG:HD2	1:F:151:GLN:O	2.18	0.44
1:F:855:GLY:O	1:F:857:THR:N	2.48	0.44
1:F:1018:ILE:HG21	1:F:1044:LEU:CD1	2.38	0.44
1:G:35:HIS:HB2	1:G:1064:SER:HB3	2.00	0.44
1:G:192:ARG:HD2	1:G:198:GLY:C	2.43	0.44
1:G:231:ALA:HB3	1:G:863:ILE:HD11	1.97	0.44
1:G:855:GLY:HA2	1:G:858:GLN:HG2	1.98	0.44
1:G:938:LEU:HD23	1:G:953:LEU:HD21	1.99	0.44
2:I:143:TRP:CD2	2:I:154:ALA:HA	2.52	0.44
3:J:310:GLU:O	3:J:313:VAL:HG12	2.18	0.44
1:A:1066:ILE:HD12	1:A:1066:ILE:N	2.33	0.44
1:B:872:GLU:HA	1:B:875:ASN:OD1	2.18	0.44
1:B:874:LEU:HD11	1:B:894:LEU:CD1	2.47	0.44
1:B:889:ASP:O	1:B:889:ASP:OD1	2.35	0.44
3:E:108:GLU:CG	3:E:200:ARG:HG3	2.47	0.44
3:E:182:VAL:HG13	3:E:279:ALA:HA	1.99	0.44
1:F:987:GLY:O	1:F:991:ILE:HG12	2.17	0.44
1:G:783:ILE:HD12	1:G:786:VAL:HG23	2.00	0.44
1:G:819:LEU:HD23	1:G:820:ASP:H	1.82	0.44
2:H:41:GLU:OE2	2:H:42:THR:HG22	2.17	0.44
3:J:66:SER:OG	3:J:67:GLN:OE1	2.35	0.44
3:J:126:ALA:O	3:J:129:LEU:HB3	2.18	0.44
1:A:982:GLN:HB2	1:B:77:ASP:OD2	2.17	0.44
2:C:63:GLU:OE2	2:C:71:ARG:NH1	2.51	0.44
2:C:164:GLN:HE21	1:F:919:PHE:HB2	1.82	0.44
3:E:165:LEU:HD21	3:J:151:VAL:HG12	1.99	0.44
3:E:173:ILE:CD1	3:J:147:PRO:HG3	2.48	0.44
1:F:247:GLU:OE2	1:F:247:GLU:CA	2.65	0.44
1:G:127:LEU:HD12	1:G:139:MET:SD	2.58	0.44
1:G:246:THR:HA	1:G:928:TYR:OH	2.17	0.44
1:G:247:GLU:O	1:G:250:GLN:HG2	2.18	0.44
2:I:121:ARG:HH22	2:I:123:GLN:CD	2.25	0.44
1:A:100:ILE:O	1:A:100:ILE:HG22	2.18	0.43
1:B:253:GLU:O	1:B:256:ARG:HG2	2.18	0.43
1:B:1085:LEU:HB2	3:E:477:ARG:HG3	1.99	0.43
2:C:136:LEU:HD23	2:C:161:LEU:HD21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:GLU:CB	2:D:70:TYR:HD2	2.30	0.43
2:D:213:LEU:O	2:D:215:ASP:N	2.48	0.43
3:E:91:ARG:O	3:E:92:ARG:HB2	2.17	0.43
3:E:437:LEU:HA	3:E:437:LEU:HD23	1.76	0.43
1:F:121:VAL:O	1:F:121:VAL:HG12	2.17	0.43
1:F:803:GLU:OE1	1:F:806:ARG:HB3	2.18	0.43
1:F:907:LEU:HD22	1:F:953:LEU:CD1	2.47	0.43
3:J:91:ARG:O	3:J:92:ARG:HB2	2.17	0.43
3:J:96:GLU:OE1	3:J:96:GLU:HA	2.17	0.43
3:J:165:LEU:HD12	3:J:165:LEU:C	2.42	0.43
3:J:266:ARG:O	3:J:270:ILE:HG13	2.18	0.43
1:A:56:LEU:CD2	1:A:60:LEU:HD22	2.48	0.43
1:A:801:MET:HE2	1:A:822:ILE:CD1	2.46	0.43
1:A:1086:GLU:HG3	1:A:1087:ARG:N	2.33	0.43
2:D:58:TYR:O	3:E:367:PRO:HG3	2.18	0.43
3:E:61:LEU:HD13	3:E:72:ILE:HD13	2.00	0.43
3:E:188:VAL:HG21	3:J:139:LEU:HD22	2.00	0.43
3:E:399:ASP:O	3:E:402:TRP:N	2.50	0.43
1:F:263:GLN:N	1:F:264:PRO:HD2	2.33	0.43
1:G:252:LEU:O	1:G:255:ALA:HB3	2.18	0.43
1:G:796:GLU:OE1	1:G:796:GLU:C	2.61	0.43
3:J:55:GLN:OE1	3:J:55:GLN:HA	2.18	0.43
3:J:125:THR:OG1	3:J:127:SER:O	2.30	0.43
1:A:955:ASP:HB3	1:A:958:PHE:HB2	2.00	0.43
1:A:1085:LEU:HD12	1:A:1085:LEU:HA	1.86	0.43
1:B:252:LEU:HD21	1:B:841:LEU:HD13	1.99	0.43
1:B:901:HIS:CE1	1:B:903:SER:CB	2.96	0.43
1:B:915:ASN:HA	1:B:918:ARG:HD2	1.98	0.43
1:B:1087:ARG:CB	3:E:477:ARG:HH11	2.31	0.43
2:C:42:THR:HG23	2:C:42:THR:O	2.18	0.43
3:E:294:ARG:HB3	3:E:294:ARG:CZ	2.49	0.43
3:E:461:ILE:HG13	3:E:461:ILE:O	2.17	0.43
1:F:54:ASP:OD2	1:F:83:TYR:OH	2.28	0.43
1:F:65:ARG:N	1:F:206:ASN:HD21	2.16	0.43
1:F:88:SER:O	1:F:88:SER:OG	2.37	0.43
1:F:828:ARG:NH2	1:F:832:LEU:HD21	2.33	0.43
1:F:890:ARG:HD3	1:F:975:ILE:CD1	2.49	0.43
1:F:957:ARG:HG3	1:F:957:ARG:HH11	1.83	0.43
1:G:62:ALA:HB2	1:G:188:LEU:HD13	1.99	0.43
1:G:65:ARG:HB2	1:G:68:LEU:HD22	2.01	0.43
1:G:217:ILE:HG13	1:G:218:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:182:LEU:HD11	2:I:186:LEU:HD11	2.01	0.43
1:A:82:SER:O	1:A:86:GLY:N	2.50	0.43
1:A:207:ARG:HH12	1:A:227:ASP:HB3	1.83	0.43
1:B:65:ARG:HB2	1:B:68:LEU:HD22	2.00	0.43
1:B:88:SER:OG	1:B:1070:ARG:NH2	2.51	0.43
1:B:939:ARG:NH1	1:B:942:CYS:HB3	2.33	0.43
1:B:967:MET:HE2	1:B:967:MET:HB3	1.95	0.43
1:B:1047:VAL:O	1:B:1047:VAL:HG23	2.17	0.43
3:E:161:LEU:CD1	3:J:157:ARG:HB3	2.45	0.43
3:E:165:LEU:HD23	3:J:155:ARG:CG	2.48	0.43
3:E:291:LEU:O	3:E:294:ARG:HG3	2.17	0.43
1:F:50:THR:OG1	4:F:1101:ADP:O1B	2.32	0.43
1:F:87:VAL:HG12	1:F:100:ILE:HG13	2.00	0.43
1:F:282:TRP:CE3	1:F:783:ILE:HD12	2.53	0.43
2:I:214:ALA:HB2	3:J:370:GLU:HG2	2.00	0.43
3:J:23:ILE:HG22	3:J:88:TRP:CH2	2.53	0.43
3:J:241:THR:HG23	3:J:245:ARG:NH1	2.33	0.43
1:A:192:ARG:HD3	1:A:199:GLU:N	2.34	0.43
1:A:798:THR:HA	1:A:801:MET:HG3	2.00	0.43
1:B:143:TRP:C	1:B:144:LEU:HD12	2.43	0.43
1:B:909:LYS:O	1:B:913:GLN:HG2	2.18	0.43
2:D:222:LEU:CD1	3:E:377:VAL:HG12	2.48	0.43
3:E:165:LEU:HD23	3:J:155:ARG:HG2	1.99	0.43
3:E:267:LEU:CD2	3:J:136:ILE:CD1	2.97	0.43
1:F:193:ASP:HA	2:H:176:SER:HB3	1.99	0.43
1:F:279:LEU:HD13	1:F:786:VAL:CG1	2.48	0.43
2:H:135:ILE:HD13	2:H:164:GLN:HG2	2.00	0.43
2:I:74:LEU:HD23	2:I:74:LEU:HA	1.81	0.43
2:I:136:LEU:HD22	2:I:206:ILE:HD11	2.00	0.43
1:A:122:ARG:HD2	1:A:151:GLN:O	2.17	0.43
1:A:824:VAL:CG2	1:A:825:TYR:N	2.81	0.43
1:B:792:ARG:CB	1:B:792:ARG:HH11	2.32	0.43
1:B:909:LYS:CB	1:B:912:ARG:HH22	2.32	0.43
1:B:933:VAL:HG12	1:B:937:GLN:HE22	1.82	0.43
3:E:62:ILE:C	3:E:65:VAL:HG13	2.43	0.43
3:E:482:LEU:H	3:E:482:LEU:CD2	2.31	0.43
1:F:80:LEU:HD11	1:F:127:LEU:HD13	2.01	0.43
1:F:242:PHE:HE1	1:F:931:LEU:HD23	1.82	0.43
1:F:805:LYS:HD2	1:F:805:LYS:HA	1.74	0.43
1:F:824:VAL:HG23	1:F:825:TYR:CD1	2.54	0.43
1:F:948:LEU:HD12	1:F:948:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:805:LYS:HE3	1:G:805:LYS:HB3	1.80	0.43
1:G:877:LEU:HD21	1:G:999:ALA:HB1	2.00	0.43
1:G:1042:PHE:O	1:G:1044:LEU:HD23	2.18	0.43
2:I:222:LEU:HD12	2:I:222:LEU:HA	1.79	0.43
3:J:369:ILE:HD12	3:J:369:ILE:O	2.19	0.43
1:B:56:LEU:CD1	1:B:60:LEU:CD2	2.97	0.43
1:B:170:GLN:O	1:B:174:GLU:HG3	2.18	0.43
1:B:172:GLU:HB2	1:B:180:THR:HG21	2.00	0.43
1:B:836:ALA:O	1:B:840:LYS:HB3	2.19	0.43
1:B:845:LEU:O	1:B:848:LEU:HG	2.19	0.43
2:C:69:LEU:HA	2:C:72:ILE:HD13	2.00	0.43
3:E:136:ILE:CD1	3:J:267:LEU:HD22	2.46	0.43
1:F:868:LEU:HD23	1:F:868:LEU:C	2.43	0.43
1:F:885:ASP:HB3	1:F:887:GLN:O	2.19	0.43
1:G:251:GLU:HG3	1:G:251:GLU:H	1.67	0.43
1:G:902:GLU:HA	1:G:905:ARG:CZ	2.48	0.43
1:G:1039:LEU:HD12	1:G:1039:LEU:HA	1.74	0.43
1:G:1085:LEU:CB	3:J:477:ARG:HH21	2.31	0.43
2:H:115:TRP:CG	2:H:124:ARG:HG2	2.54	0.43
2:H:131:LEU:O	2:H:135:ILE:HG13	2.18	0.43
3:J:40:LEU:HB3	3:J:48:ILE:HG13	2.01	0.43
3:J:240:ASN:OD1	3:J:240:ASN:O	2.37	0.43
1:A:282:TRP:CE3	1:A:783:ILE:HD12	2.54	0.43
1:A:940:ASP:OD2	1:A:940:ASP:C	2.62	0.43
1:B:144:LEU:HB2	1:B:156:TRP:CH2	2.52	0.43
2:C:43:ARG:HD2	2:C:43:ARG:HA	1.80	0.43
2:D:66:LYS:HD2	2:D:66:LYS:N	2.34	0.43
3:E:136:ILE:HD11	3:J:267:LEU:CD2	2.48	0.43
1:F:785:ARG:CZ	1:F:785:ARG:HB3	2.47	0.43
1:F:966:VAL:CG1	1:F:976:GLU:HB3	2.48	0.43
2:I:94:ASP:OD2	2:I:97:ARG:HB2	2.18	0.43
1:A:266:ALA:O	1:A:270:GLU:HG3	2.18	0.43
1:B:217:ILE:HD11	1:B:962:PHE:C	2.44	0.43
1:B:1031:VAL:O	1:B:1035:ILE:CD1	2.59	0.43
1:B:1038:ALA:HA	1:B:1041:GLU:CD	2.44	0.43
2:C:94:ASP:OD2	2:C:97:ARG:HG3	2.19	0.43
2:D:74:LEU:HD23	2:D:74:LEU:HA	1.79	0.43
1:F:14:ILE:CD1	1:F:16:THR:HG22	2.47	0.43
1:F:982:GLN:HB3	1:G:77:ASP:OD2	2.19	0.43
1:G:252:LEU:HA	1:G:840:LYS:NZ	2.34	0.43
1:G:890:ARG:HG3	1:G:890:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:THR:O	2:H:42:THR:HG23	2.18	0.43
2:H:158:ILE:HD13	2:H:158:ILE:HA	1.76	0.43
3:J:131:THR:OG1	3:J:134:ARG:NH2	2.51	0.43
3:J:204:ASP:OD1	3:J:204:ASP:N	2.52	0.43
3:J:294:ARG:HG2	3:J:294:ARG:HH11	1.84	0.43
1:A:49:LYS:HB3	1:A:1049:ILE:CG2	2.49	0.43
1:B:796:GLU:C	1:B:796:GLU:OE1	2.62	0.43
1:B:889:ASP:O	1:B:889:ASP:CG	2.61	0.43
1:B:890:ARG:HG3	1:B:890:ARG:NH1	2.34	0.43
3:E:148:ALA:HA	3:E:151:VAL:HG23	2.00	0.43
3:E:187:ASP:C	3:E:187:ASP:OD2	2.61	0.43
1:F:100:ILE:O	1:F:100:ILE:HG22	2.18	0.43
1:F:805:LYS:HZ1	1:F:813:VAL:HA	1.83	0.43
1:G:829:LEU:C	1:G:829:LEU:HD13	2.43	0.43
2:H:128:GLU:HG3	2:H:185:LEU:CD2	2.46	0.43
1:A:851:SER:O	1:A:852:SER:CB	2.65	0.42
1:B:105:LYS:HE3	1:B:130:ASP:CA	2.45	0.42
1:B:877:LEU:O	1:B:877:LEU:HD22	2.19	0.42
1:B:902:GLU:HA	1:B:905:ARG:CZ	2.49	0.42
1:B:1059:ARG:HB2	3:E:443:LEU:HD22	2.01	0.42
2:D:54:GLU:HA	2:D:54:GLU:OE1	2.19	0.42
3:E:54:ILE:HD13	3:E:82:SER:HA	2.01	0.42
3:E:74:GLN:HE21	3:E:74:GLN:C	2.24	0.42
1:G:34:ILE:HG23	1:G:39:THR:HG21	2.00	0.42
1:G:146:SER:HA	1:G:178:LEU:HD23	2.01	0.42
2:I:143:TRP:O	2:I:146:GLU:HG3	2.18	0.42
3:J:227:ILE:HD11	3:J:317:MET:CB	2.37	0.42
1:A:30:HIS:HE1	3:E:387:LEU:HD22	1.83	0.42
1:A:132:THR:O	1:A:132:THR:CG2	2.68	0.42
1:A:263:GLN:N	1:A:264:PRO:HD2	2.33	0.42
1:A:828:ARG:HD2	1:A:828:ARG:HA	1.82	0.42
1:A:848:LEU:HD21	1:A:927:HIS:ND1	2.34	0.42
1:A:957:ARG:HH11	1:A:957:ARG:HG3	1.84	0.42
1:B:107:VAL:CG2	1:B:160:TYR:HE1	2.25	0.42
1:B:837:LEU:HD23	1:B:837:LEU:HA	1.83	0.42
1:B:915:ASN:C	1:B:918:ARG:HD2	2.43	0.42
1:B:938:LEU:HD23	1:B:953:LEU:HD21	2.00	0.42
2:C:124:ARG:CB	3:E:353:GLU:OE2	2.66	0.42
3:E:39:THR:HG21	3:J:5:THR:CG2	2.49	0.42
3:E:470:LEU:HD13	3:E:470:LEU:C	2.44	0.42
1:F:18:ILE:HD11	1:F:56:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:892:LEU:HD23	1:F:892:LEU:C	2.44	0.42
1:F:1016:GLY:O	1:F:1045:HIS:N	2.52	0.42
1:A:26:PHE:HB3	1:A:30:HIS:CD2	2.54	0.42
1:A:897:LYS:O	1:A:960:LEU:HB2	2.20	0.42
1:B:148:ASN:HB3	1:B:151:GLN:NE2	2.34	0.42
1:B:871:GLU:OE2	1:B:871:GLU:C	2.63	0.42
2:C:44:THR:O	2:C:49:ARG:NE	2.53	0.42
2:C:45:LEU:CD1	2:C:48:ILE:HD12	2.32	0.42
2:C:60:LEU:HD12	2:C:99:LEU:HD11	2.00	0.42
2:C:121:ARG:CG	2:C:122:ARG:H	2.32	0.42
2:C:155:GLN:HG2	2:C:205:VAL:CG2	2.49	0.42
2:C:158:ILE:HD12	2:C:186:LEU:CD1	2.49	0.42
3:E:19:HIS:ND1	3:J:117:LEU:CD2	2.82	0.42
3:E:282:ARG:NH1	3:E:282:ARG:HB3	2.34	0.42
1:F:115:GLU:CG	1:F:120:GLN:HG3	2.48	0.42
1:G:975:ILE:HG22	1:G:976:GLU:OE2	2.19	0.42
2:H:223:LEU:HD12	2:H:223:LEU:HA	1.87	0.42
3:J:74:GLN:HE21	3:J:74:GLN:C	2.24	0.42
1:A:907:LEU:HB2	1:A:953:LEU:HD11	2.00	0.42
1:A:979:THR:O	1:A:979:THR:HG23	2.19	0.42
1:B:209:ALA:HA	1:B:1019:ILE:O	2.20	0.42
1:B:212:LYS:C	1:B:213:GLN:HG2	2.44	0.42
1:B:878:ASN:CG	1:B:893:ARG:HB2	2.44	0.42
1:B:895:ASP:OD1	1:B:963:ALA:HB3	2.19	0.42
1:B:975:ILE:HG22	1:B:976:GLU:OE2	2.18	0.42
2:D:70:TYR:HE1	2:D:100:LEU:HD21	1.84	0.42
3:E:148:ALA:HA	3:E:151:VAL:CG2	2.49	0.42
3:E:279:ALA:C	3:E:280:LEU:HD23	2.45	0.42
1:G:107:VAL:HG22	1:G:128:TRP:CB	2.49	0.42
1:G:815:ALA:HB1	1:G:821:ASP:OD1	2.20	0.42
2:H:124:ARG:HB2	3:J:353:GLU:CG	2.47	0.42
3:J:4:ASN:C	3:J:4:ASN:OD1	2.61	0.42
3:J:144:ASN:ND2	3:J:150:ARG:HG3	2.34	0.42
1:A:885:ASP:HB3	1:A:887:GLN:O	2.20	0.42
1:A:901:HIS:HD2	1:A:948:LEU:HG	1.84	0.42
1:B:1055:MET:HB2	3:E:444:GLU:CD	2.44	0.42
3:E:16:LYS:O	3:E:16:LYS:HD2	2.19	0.42
3:E:356:LEU:HA	3:E:356:LEU:HD23	1.75	0.42
1:F:30:HIS:HE1	3:J:387:LEU:HD22	1.85	0.42
1:F:268:SER:OG	1:F:797:LEU:HD22	2.20	0.42
1:F:279:LEU:HD22	1:F:787:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:797:LEU:O	1:F:801:MET:HG3	2.19	0.42
1:F:1056:ARG:HE	3:J:407:GLY:N	2.10	0.42
1:G:69:ALA:HB2	1:G:1021:ASP:HB3	2.01	0.42
1:G:81:ILE:HD11	1:G:135:SER:C	2.45	0.42
1:G:126:LEU:HD11	1:G:157:LEU:HD13	2.02	0.42
1:G:1018:ILE:HG23	1:G:1046:ALA:HB2	2.02	0.42
1:G:1085:LEU:HB2	3:J:477:ARG:HH21	1.84	0.42
2:H:47:LYS:NZ	2:H:47:LYS:CB	2.82	0.42
2:H:73:VAL:CG1	2:H:80:VAL:HG21	2.33	0.42
2:H:216:PRO:HD3	3:J:328:VAL:HG23	2.00	0.42
3:J:470:LEU:HD13	3:J:470:LEU:C	2.43	0.42
1:B:127:LEU:HD13	1:B:139:MET:HE3	2.00	0.42
1:B:997:LEU:HA	1:B:1000:SER:OG	2.20	0.42
3:E:62:ILE:HA	3:E:65:VAL:HG13	2.00	0.42
3:E:173:ILE:H	3:E:173:ILE:HG12	1.75	0.42
1:F:797:LEU:HD12	1:F:801:MET:HE2	2.00	0.42
1:G:49:LYS:HB2	1:G:1049:ILE:HG21	2.00	0.42
1:G:217:ILE:HA	1:G:220:ILE:HB	2.01	0.42
2:H:121:ARG:CG	2:H:122:ARG:H	2.32	0.42
2:H:194:LEU:HD21	2:H:213:LEU:HD22	2.02	0.42
3:J:153:THR:O	3:J:156:ARG:HG2	2.20	0.42
3:J:191:LEU:HD23	3:J:191:LEU:HA	1.76	0.42
3:J:421:LEU:C	3:J:489:SER:HB2	2.44	0.42
1:A:15:LEU:CD2	1:A:34:ILE:HD12	2.49	0.42
1:A:217:ILE:HG21	1:A:964:VAL:HG23	2.01	0.42
1:A:264:PRO:HB2	1:A:800:ARG:HD2	2.02	0.42
1:B:107:VAL:HG22	1:B:128:TRP:HB2	2.01	0.42
1:B:819:LEU:C	1:B:822:ILE:HG12	2.45	0.42
1:B:842:ASN:O	1:B:845:LEU:HG	2.20	0.42
2:C:74:LEU:HD23	2:C:74:LEU:HA	1.82	0.42
3:E:324:GLU:H	3:E:324:GLU:CD	2.28	0.42
1:F:895:ASP:OD1	1:F:896:THR:N	2.52	0.42
1:G:234:ARG:HA	1:G:237:GLU:CD	2.45	0.42
1:G:889:ASP:O	1:G:889:ASP:CG	2.63	0.42
1:G:955:ASP:CG	1:G:957:ARG:HH21	2.27	0.42
2:I:209:ILE:CD1	3:J:369:ILE:HG21	2.33	0.42
3:J:421:LEU:CB	3:J:489:SER:HB2	2.49	0.42
1:A:893:ARG:HE	1:A:893:ARG:HB3	1.72	0.42
1:B:21:PHE:HE1	1:B:29:LEU:HB2	1.84	0.42
1:B:242:PHE:CD2	1:B:935:VAL:CG2	3.03	0.42
1:B:799:LYS:O	1:B:802:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:GLY:C	1:B:856:VAL:HG23	2.44	0.42
1:B:955:ASP:CG	1:B:957:ARG:HH21	2.27	0.42
1:B:963:ALA:HB1	1:B:978:ARG:NH1	2.35	0.42
3:E:162:GLU:N	3:J:158:ILE:HD11	2.35	0.42
3:E:466:GLU:C	3:E:467:PHE:CD2	2.98	0.42
3:E:476:ARG:HB3	3:E:478:TRP:CZ2	2.54	0.42
1:F:219:GLU:O	1:F:223:GLU:HB2	2.19	0.42
1:F:224:LEU:HD21	1:F:997:LEU:HD13	2.01	0.42
1:G:811:ALA:HB1	1:G:828:ARG:HE	1.84	0.42
1:G:881:MET:HE1	1:G:893:ARG:CA	2.45	0.42
1:G:1054:GLU:CD	1:G:1057:LEU:HD21	2.45	0.42
1:G:1087:ARG:HG3	3:J:477:ARG:NH1	2.35	0.42
2:I:132:LEU:O	2:I:136:LEU:HG	2.19	0.42
3:J:282:ARG:NH1	3:J:282:ARG:HB3	2.35	0.42
1:A:805:LYS:CD	1:A:812:LEU:HB3	2.50	0.42
1:B:62:ALA:CB	1:B:188:LEU:HD13	2.50	0.42
2:C:57:LYS:HE3	2:C:58:TYR:CZ	2.55	0.42
2:C:94:ASP:HB2	2:C:212:HIS:NE2	2.34	0.42
2:D:70:TYR:CE1	2:D:100:LEU:HD21	2.55	0.42
3:E:61:LEU:O	3:E:72:ILE:HG21	2.20	0.42
1:F:274:LYS:O	1:F:274:LYS:HD3	2.20	0.42
1:G:842:ASN:HA	1:G:845:LEU:HD21	2.02	0.42
1:G:916:ALA:HA	1:G:919:PHE:CZ	2.55	0.42
2:I:47:LYS:HE2	2:I:47:LYS:CA	2.44	0.42
1:A:1057:LEU:HG	1:A:1058:LEU:HD22	2.00	0.42
1:B:855:GLY:HA2	1:B:858:GLN:NE2	2.27	0.42
1:B:876:GLU:HB3	1:B:1003:TYR:CZ	2.55	0.42
2:D:227:ARG:CZ	2:D:227:ARG:HB2	2.50	0.42
3:E:39:THR:HA	3:J:8:ARG:HH22	1.85	0.42
1:F:20:LEU:HD23	1:F:110:ILE:HG22	2.01	0.42
1:F:26:PHE:HB3	1:F:30:HIS:CD2	2.55	0.42
1:F:797:LEU:HD12	1:F:801:MET:CE	2.49	0.42
2:I:70:TYR:HD2	2:I:100:LEU:CD1	2.33	0.42
2:I:158:ILE:HD11	2:I:183:LEU:CD2	2.50	0.42
1:A:79:ASP:C	1:A:79:ASP:OD1	2.63	0.41
1:B:46:GLY:O	1:B:1070:ARG:HB3	2.20	0.41
1:B:143:TRP:HE1	1:B:184:LYS:N	2.18	0.41
1:B:988:GLU:O	1:B:992:ILE:HD13	2.19	0.41
3:E:4:ASN:OD1	3:E:4:ASN:C	2.63	0.41
3:E:241:THR:N	3:E:242:PRO:CD	2.83	0.41
3:E:413:LEU:HD12	3:E:417:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:TRP:NE1	1:F:140:LYS:HB2	2.35	0.41
1:F:851:SER:O	1:F:852:SER:CB	2.68	0.41
1:G:184:LYS:HG2	1:G:188:LEU:HG	2.02	0.41
1:G:217:ILE:HD11	1:G:963:ALA:N	2.35	0.41
1:G:945:ASN:O	1:G:951:LYS:HG2	2.19	0.41
1:G:997:LEU:HD12	1:G:1000:SER:OG	2.20	0.41
2:H:62:GLU:CG	2:H:99:LEU:HD12	2.50	0.41
1:B:847:TYR:O	1:B:851:SER:OG	2.30	0.41
2:C:146:GLU:O	2:C:146:GLU:CD	2.63	0.41
3:E:470:LEU:HD13	3:E:471:SER:C	2.45	0.41
1:F:27:HIS:O	1:F:30:HIS:NE2	2.52	0.41
1:F:132:THR:O	1:F:132:THR:CG2	2.68	0.41
1:F:906:THR:HA	1:F:909:LYS:HD3	2.02	0.41
1:F:994:SER:O	1:F:998:THR:OG1	2.33	0.41
1:G:91:GLY:HA3	1:G:99:HIS:ND1	2.34	0.41
1:G:181:TYR:CD2	1:G:187:TYR:HA	2.54	0.41
1:G:196:GLU:HB3	1:G:1007:PRO:HB3	2.01	0.41
1:G:879:GLU:O	1:G:883:ARG:HG3	2.18	0.41
1:G:957:ARG:H	1:G:957:ARG:HG3	1.71	0.41
2:H:119:LEU:HD23	3:J:363:VAL:HG22	2.02	0.41
2:I:213:LEU:HD13	2:I:219:LEU:HD11	2.02	0.41
3:J:419:GLN:CG	3:J:423:LYS:HE2	2.48	0.41
1:A:15:LEU:HD11	1:A:17:ARG:O	2.20	0.41
1:A:279:LEU:HD13	1:A:786:VAL:HG12	2.02	0.41
1:A:806:ARG:CG	1:B:806:ARG:HH21	2.33	0.41
1:A:851:SER:O	1:A:931:LEU:CD2	2.68	0.41
1:B:787:LYS:HD3	1:B:787:LYS:C	2.45	0.41
1:B:790:LEU:HD23	1:B:790:LEU:O	2.19	0.41
1:B:1087:ARG:HB3	3:E:477:ARG:NH1	2.35	0.41
2:D:185:LEU:HD23	2:D:185:LEU:HA	1.84	0.41
3:E:158:ILE:HG12	3:J:161:LEU:HD22	1.97	0.41
1:G:228:ASP:OD1	1:G:229:HIS:N	2.53	0.41
1:G:875:ASN:OD1	1:G:875:ASN:N	2.51	0.41
1:G:914:LEU:HD23	1:G:918:ARG:HE	1.85	0.41
1:G:967:MET:HE2	1:G:973:ASN:C	2.45	0.41
2:H:74:LEU:HD23	2:H:74:LEU:HA	1.82	0.41
3:J:7:GLN:O	3:J:10:GLU:HB2	2.21	0.41
3:J:411:GLU:C	3:J:411:GLU:OE1	2.62	0.41
1:A:261:SER:O	1:A:264:PRO:HG2	2.20	0.41
1:B:1031:VAL:C	1:B:1035:ILE:HD12	2.45	0.41
2:C:117:HIS:HE1	2:C:119:LEU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:LEU:HD23	3:E:85:LEU:HA	1.87	0.41
3:E:217:ILE:CG2	3:E:227:ILE:HD11	2.47	0.41
3:E:443:LEU:HA	3:E:446:PHE:HD2	1.85	0.41
1:F:837:LEU:HD23	1:F:837:LEU:HA	1.85	0.41
1:G:40:ALA:O	1:G:1065:ALA:HA	2.20	0.41
1:G:71:THR:CG2	1:G:74:HIS:HB2	2.49	0.41
1:G:983:GLY:H	1:G:988:GLU:N	2.14	0.41
1:G:1007:PRO:HD2	1:G:1010:SER:HB3	2.02	0.41
2:I:66:LYS:HD2	2:I:66:LYS:N	2.34	0.41
2:I:144:GLU:CD	2:I:149:THR:HA	2.45	0.41
2:I:198:PRO:HD2	2:I:198:PRO:O	2.19	0.41
2:I:209:ILE:CG1	3:J:369:ILE:HG12	2.50	0.41
3:J:293:LYS:HB2	3:J:293:LYS:HE3	1.61	0.41
1:A:81:ILE:HD12	1:A:129:PHE:HZ	1.86	0.41
1:A:269:TRP:CE2	1:A:822:ILE:HG21	2.55	0.41
1:B:57:MET:HE3	1:B:206:ASN:HA	2.01	0.41
1:B:91:GLY:HA3	1:B:99:HIS:ND1	2.36	0.41
2:C:148:GLY:HA2	3:E:312:ASP:OD2	2.21	0.41
3:E:34:LEU:HD23	3:E:34:LEU:HA	1.74	0.41
3:E:417:THR:HG21	3:E:449:TRP:HE1	1.86	0.41
1:F:902:GLU:C	1:F:902:GLU:OE1	2.64	0.41
1:F:906:THR:HG22	1:F:937:GLN:HE22	1.83	0.41
1:F:1040:ARG:HG2	1:F:1040:ARG:NH1	2.35	0.41
1:G:195:PHE:C	1:G:1014:LEU:HD23	2.45	0.41
1:G:783:ILE:HG23	1:G:784:GLU:OE1	2.20	0.41
1:G:894:LEU:HA	1:G:964:VAL:HA	2.02	0.41
2:H:135:ILE:CG2	2:H:164:GLN:HG2	2.50	0.41
2:H:135:ILE:HG23	2:H:164:GLN:HG2	2.03	0.41
2:H:153:GLN:O	2:H:154:ALA:C	2.64	0.41
2:I:179:ARG:HG3	2:I:179:ARG:HH11	1.85	0.41
3:J:279:ALA:C	3:J:280:LEU:HD23	2.46	0.41
3:J:487:LEU:CG	3:J:492:LEU:HD11	2.36	0.41
1:A:39:THR:HG21	1:A:1066:ILE:CD1	2.50	0.41
1:A:803:GLU:O	1:A:806:ARG:HB3	2.20	0.41
1:A:839:GLU:O	1:A:840:LYS:C	2.64	0.41
2:C:104:VAL:HG11	2:C:114:GLU:HB2	2.02	0.41
2:C:158:ILE:HD13	2:C:158:ILE:HA	1.76	0.41
3:E:67:GLN:HA	3:E:67:GLN:NE2	2.35	0.41
3:E:455:GLU:CG	3:E:495:ILE:HD12	2.40	0.41
1:G:876:GLU:HB3	1:G:1003:TYR:CZ	2.55	0.41
2:I:90:ASP:OD1	2:I:91:ILE:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:122:ARG:NH2	3:J:373:ARG:HH21	2.17	0.41
3:J:459:GLU:HG2	3:J:460:VAL:N	2.35	0.41
1:A:37:ASP:HB2	1:A:1063:ARG:HG2	2.03	0.41
1:A:967:MET:HE2	1:A:972:GLY:O	2.21	0.41
1:B:194:PHE:C	1:B:194:PHE:CD2	2.97	0.41
1:B:891:TYR:CE2	1:B:967:MET:HB2	2.56	0.41
1:B:891:TYR:OH	1:B:967:MET:SD	2.78	0.41
1:B:967:MET:HE2	1:B:973:ASN:C	2.46	0.41
2:C:45:LEU:HD13	2:C:48:ILE:CD1	2.33	0.41
2:C:153:GLN:O	2:C:154:ALA:C	2.63	0.41
3:E:61:LEU:HD13	3:E:72:ILE:CD1	2.51	0.41
3:E:256:GLN:HB3	3:E:259:GLU:OE1	2.20	0.41
3:E:369:ILE:HD12	3:E:369:ILE:O	2.21	0.41
3:E:417:THR:C	3:E:421:LEU:HD12	2.45	0.41
1:F:143:TRP:CH2	1:F:184:LYS:HE3	2.56	0.41
1:F:887:GLN:O	1:F:888:PRO:C	2.63	0.41
1:G:273:GLN:O	1:G:277:ARG:HG3	2.21	0.41
1:G:842:ASN:HA	1:G:845:LEU:HG	2.02	0.41
1:G:953:LEU:HD23	1:G:954:LEU:HD11	2.01	0.41
2:I:197:SER:HB3	2:I:198:PRO:HD3	2.02	0.41
3:J:50:LEU:HB2	3:J:99:GLY:O	2.20	0.41
3:J:338:LEU:O	3:J:341:LYS:HG2	2.21	0.41
3:J:347:GLN:HG3	3:J:351:LYS:CG	2.50	0.41
1:A:272:TYR:N	1:A:793:LEU:HD23	2.36	0.41
1:A:984:GLY:O	1:A:989:LYS:NZ	2.53	0.41
1:A:985:SER:HB2	4:B:1101:ADP:PB	2.61	0.41
1:B:42:ILE:HD12	1:B:1055:MET:CE	2.32	0.41
1:B:53:VAL:HG22	1:B:1019:ILE:CG2	2.49	0.41
1:B:78:ARG:HG2	4:B:1101:ADP:N6	2.36	0.41
1:B:102:ARG:CG	1:B:106:THR:HG21	2.51	0.41
3:E:8:ARG:HH22	3:J:39:THR:HA	1.86	0.41
3:E:131:THR:CB	3:E:134:ARG:HH21	2.34	0.41
3:E:211:ARG:CZ	3:E:211:ARG:HB2	2.51	0.41
1:F:2:ASN:HA	1:F:5:SER:OG	2.20	0.41
1:F:185:LYS:HA	1:F:185:LYS:HE2	2.02	0.41
1:F:955:ASP:HB3	1:F:958:PHE:HB2	2.02	0.41
1:G:1047:VAL:O	1:G:1047:VAL:HG23	2.20	0.41
2:H:46:GLN:HA	2:H:49:ARG:NH1	2.36	0.41
2:H:158:ILE:HD12	2:H:186:LEU:CD1	2.51	0.41
1:A:832:LEU:CD2	1:A:836:ALA:HB3	2.49	0.41
1:A:985:SER:OG	4:B:1101:ADP:O1B	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:GLY:O	1:A:1045:HIS:N	2.52	0.41
1:B:40:ALA:HB2	1:B:1058:LEU:HD13	2.03	0.41
1:B:217:ILE:HD11	1:B:963:ALA:N	2.35	0.41
1:B:221:PHE:O	1:B:226:LEU:HB2	2.21	0.41
1:B:242:PHE:CD1	1:B:242:PHE:C	2.97	0.41
1:B:792:ARG:HH11	1:B:792:ARG:HB3	1.86	0.41
1:B:914:LEU:CD1	1:B:931:LEU:HD22	2.51	0.41
1:B:1007:PRO:HD2	1:B:1010:SER:HB3	2.03	0.41
2:C:99:LEU:HD13	2:C:208:PRO:HB2	2.02	0.41
2:D:215:ASP:OD2	2:D:218:ASN:OD1	2.39	0.41
3:E:40:LEU:HB3	3:E:48:ILE:HG13	2.02	0.41
3:E:43:LYS:HG3	3:E:44:SER:N	2.35	0.41
3:E:140:GLU:HG3	3:J:266:ARG:HB3	2.03	0.41
3:E:261:LYS:N	3:E:261:LYS:HD3	2.36	0.41
3:E:294:ARG:HG2	3:E:294:ARG:HH11	1.86	0.41
1:F:905:ARG:O	1:F:909:LYS:HG3	2.21	0.41
1:G:10:LYS:HB3	1:G:10:LYS:HE3	1.71	0.41
1:G:21:PHE:O	1:G:108:THR:HG23	2.21	0.41
1:G:27:HIS:CE1	1:G:101:ALA:HB1	2.56	0.41
1:G:81:ILE:HA	1:G:84:VAL:CG2	2.51	0.41
1:G:107:VAL:HG11	1:G:160:TYR:HE1	1.81	0.41
1:G:1085:LEU:HD12	3:J:477:ARG:HE	1.85	0.41
2:I:137:ARG:NH2	2:I:216:PRO:HB3	2.36	0.41
2:I:168:TYR:HB3	2:I:226:LEU:HD22	2.02	0.41
3:J:61:LEU:O	3:J:72:ILE:HG21	2.21	0.41
3:J:165:LEU:O	3:J:168:ALA:N	2.54	0.41
3:J:455:GLU:CG	3:J:495:ILE:HD12	2.46	0.41
1:A:27:HIS:NE2	1:A:1073:GLN:O	2.54	0.41
1:A:797:LEU:O	1:A:801:MET:CG	2.69	0.41
1:A:1018:ILE:HD11	1:A:1039:LEU:CD1	2.50	0.41
1:B:830:GLN:HA	1:B:833:THR:OG1	2.20	0.41
1:B:893:ARG:HD3	1:B:967:MET:CG	2.50	0.41
1:B:1014:LEU:HD12	1:B:1014:LEU:HA	1.85	0.41
2:C:51:ALA:HB1	2:C:73:VAL:HG22	2.03	0.41
2:C:70:TYR:CE2	2:C:100:LEU:HD21	2.46	0.41
2:C:71:ARG:HG2	2:C:71:ARG:HH11	1.86	0.41
2:D:60:LEU:HA	2:D:100:LEU:O	2.21	0.41
2:D:223:LEU:HD12	2:D:223:LEU:HA	1.77	0.41
1:F:982:GLN:CD	1:F:982:GLN:H	2.29	0.41
1:G:204:LEU:HG	1:G:1001:LEU:HD13	2.02	0.41
1:G:802:SER:OG	1:G:803:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:869:VAL:CA	1:G:872:GLU:HG2	2.47	0.41
2:I:74:LEU:CD2	2:I:93:ILE:HD12	2.52	0.41
3:J:16:LYS:O	3:J:16:LYS:HD2	2.20	0.41
3:J:210:ASP:OD1	3:J:214:ARG:NE	2.49	0.41
1:A:836:ALA:O	1:A:840:LYS:CG	2.67	0.40
1:A:982:GLN:CD	1:A:982:GLN:H	2.28	0.40
1:B:81:ILE:HD11	1:B:135:SER:C	2.46	0.40
1:B:146:SER:CB	1:B:178:LEU:HD23	2.48	0.40
2:C:209:ILE:HD12	2:C:209:ILE:HA	1.98	0.40
2:D:61:LEU:HD12	2:D:61:LEU:HA	1.92	0.40
2:D:209:ILE:HD11	3:E:369:ILE:HB	2.03	0.40
1:F:122:ARG:HB2	1:F:122:ARG:NH1	2.36	0.40
1:F:991:ILE:HD12	1:F:1035:ILE:HD11	2.03	0.40
1:G:34:ILE:HD12	1:G:34:ILE:N	2.36	0.40
1:G:85:ARG:NH2	1:G:134:SER:OG	2.54	0.40
1:G:894:LEU:HD23	1:G:894:LEU:N	2.35	0.40
1:A:970:GLN:OE1	1:A:971:SER:N	2.53	0.40
1:A:1050:THR:HG21	1:A:1058:LEU:CD2	2.51	0.40
1:B:34:ILE:N	1:B:34:ILE:HD12	2.36	0.40
1:B:113:THR:HG22	1:B:122:ARG:CG	2.44	0.40
1:B:940:ASP:OD1	1:B:941:ALA:N	2.54	0.40
1:B:1011:ARG:N	1:B:1011:ARG:HD3	2.36	0.40
2:C:45:LEU:H	2:C:45:LEU:CD1	2.17	0.40
2:C:127:LEU:HD23	2:C:127:LEU:HA	1.95	0.40
3:E:136:ILE:CD1	3:J:267:LEU:CD2	3.00	0.40
3:E:182:VAL:HG13	3:E:279:ALA:CA	2.51	0.40
1:F:27:HIS:O	3:J:387:LEU:HD11	2.22	0.40
1:F:806:ARG:NH1	1:G:806:ARG:HD2	2.36	0.40
1:F:893:ARG:HE	1:F:893:ARG:HB3	1.71	0.40
1:G:128:TRP:HH2	1:G:142:LEU:HB2	1.86	0.40
1:G:235:ALA:CB	1:G:954:LEU:HD21	2.50	0.40
1:G:801:MET:SD	1:G:817:ALA:HA	2.62	0.40
1:G:914:LEU:CD1	1:G:931:LEU:HD22	2.52	0.40
2:H:138:GLN:O	2:H:141:VAL:HG12	2.21	0.40
2:I:78:GLU:O	2:I:81:THR:HG22	2.21	0.40
3:J:465:ARG:NH2	3:J:481:ASN:O	2.48	0.40
3:J:480:PHE:HB3	3:J:482:LEU:CD1	2.52	0.40
1:A:268:SER:CB	1:A:797:LEU:HD22	2.50	0.40
1:A:815:ALA:CB	1:A:824:VAL:HG21	2.51	0.40
1:B:85:ARG:NH2	1:B:134:SER:OG	2.54	0.40
1:B:842:ASN:HA	1:B:845:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:430:LEU:HG	3:E:485:THR:HG21	2.02	0.40
3:E:461:ILE:HD11	3:E:484:THR:HG21	2.02	0.40
1:F:970:GLN:OE1	1:F:971:SER:N	2.54	0.40
1:F:991:ILE:HD12	1:F:1035:ILE:CD1	2.52	0.40
1:G:195:PHE:HD2	1:G:1014:LEU:HG	1.86	0.40
1:G:238:VAL:HG21	1:G:856:VAL:HG22	2.01	0.40
1:G:874:LEU:HD22	1:G:894:LEU:HG	2.03	0.40
3:J:1:MET:HE3	3:J:1:MET:HB3	1.99	0.40
1:A:65:ARG:HB3	1:A:68:LEU:HD13	2.02	0.40
1:B:958:PHE:CD1	1:B:958:PHE:N	2.89	0.40
3:E:50:LEU:HD21	3:E:86:ARG:CZ	2.52	0.40
3:E:267:LEU:O	3:E:271:LEU:CD1	2.70	0.40
3:E:424:GLU:HB3	3:E:426:ARG:HG2	2.03	0.40
1:F:68:LEU:CD2	1:F:207:ARG:HA	2.52	0.40
1:F:897:LYS:O	1:F:960:LEU:HB2	2.21	0.40
1:F:966:VAL:HG12	1:F:976:GLU:O	2.22	0.40
1:F:1024:PHE:CZ	1:F:1036:ILE:HD11	2.56	0.40
1:G:17:ARG:HA	1:G:32:ALA:O	2.21	0.40
1:G:60:LEU:HD22	1:G:60:LEU:N	2.36	0.40
1:G:887:GLN:CB	1:G:888:PRO:HD2	2.37	0.40
2:H:126:ASN:HA	3:J:352:GLN:O	2.21	0.40
2:I:109:THR:C	2:I:112:GLN:HG2	2.46	0.40
2:I:132:LEU:HD21	2:I:186:LEU:HD23	2.02	0.40
3:J:459:GLU:OE2	3:J:461:ILE:HG13	2.21	0.40
3:J:469:GLU:OE1	3:J:479:ARG:HB2	2.22	0.40
1:A:172:GLU:HA	1:A:178:LEU:HD23	2.03	0.40
1:A:860:LEU:HD12	1:A:911:GLN:OE1	2.21	0.40
1:A:1040:ARG:HG2	1:A:1040:ARG:NH1	2.37	0.40
1:B:59:LEU:HD23	1:B:110:ILE:HD11	2.03	0.40
1:B:217:ILE:O	1:B:220:ILE:HB	2.21	0.40
1:B:242:PHE:HZ	1:B:932:GLN:CG	2.33	0.40
1:B:994:SER:O	1:B:998:THR:HG23	2.21	0.40
2:D:143:TRP:CD1	2:D:143:TRP:C	2.99	0.40
2:D:144:GLU:CD	2:D:149:THR:HA	2.47	0.40
3:E:7:GLN:O	3:E:11:ASN:OD1	2.38	0.40
3:E:173:ILE:HG22	3:J:150:ARG:HD3	2.03	0.40
1:F:48:GLY:CA	1:F:1068:VAL:HG11	2.51	0.40
1:F:56:LEU:HD23	1:F:56:LEU:C	2.47	0.40
1:F:275:GLN:HB3	1:F:790:LEU:HD21	2.02	0.40
2:H:125:LEU:O	3:J:354:VAL:HG22	2.21	0.40
2:I:165:LEU:HD23	2:I:165:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:226:LEU:HD23	2:I:226:LEU:HA	1.79	0.40
3:J:97:ARG:O	3:J:98:ASP:HB3	2.21	0.40
3:J:189:TYR:CD1	3:J:189:TYR:C	2.99	0.40
3:J:356:LEU:HD23	3:J:356:LEU:HA	1.88	0.40
3:J:477:ARG:HB3	3:J:477:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/1096 (54%)	557 (94%)	35 (6%)	1 (0%)	43	74
1	B	593/1096 (54%)	557 (94%)	32 (5%)	4 (1%)	18	52
1	F	593/1096 (54%)	557 (94%)	35 (6%)	1 (0%)	43	74
1	G	593/1096 (54%)	565 (95%)	26 (4%)	2 (0%)	36	66
2	C	193/250 (77%)	178 (92%)	15 (8%)	0	100	100
2	D	193/250 (77%)	182 (94%)	11 (6%)	0	100	100
2	H	193/250 (77%)	179 (93%)	14 (7%)	0	100	100
2	I	193/250 (77%)	181 (94%)	12 (6%)	0	100	100
3	E	496/554 (90%)	471 (95%)	25 (5%)	0	100	100
3	J	496/554 (90%)	471 (95%)	25 (5%)	0	100	100
All	All	4136/6492 (64%)	3898 (94%)	230 (6%)	8 (0%)	44	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	SER
1	B	1087	ARG

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Mol	Chain	Res	Type
1	F	852	SER
1	G	1087	ARG
1	B	891	TYR
1	G	891	TYR
1	B	212	LYS
1	B	856	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/929 (54%)	497 (99%)	4 (1%)	73	77
1	B	501/929 (54%)	499 (100%)	2 (0%)	84	82
1	F	501/929 (54%)	501 (100%)	0	100	100
1	G	501/929 (54%)	498 (99%)	3 (1%)	78	80
2	C	171/218 (78%)	169 (99%)	2 (1%)	63	73
2	D	171/218 (78%)	169 (99%)	2 (1%)	63	73
2	H	171/218 (78%)	170 (99%)	1 (1%)	78	80
2	I	171/218 (78%)	171 (100%)	0	100	100
3	E	435/474 (92%)	434 (100%)	1 (0%)	87	85
3	J	435/474 (92%)	433 (100%)	2 (0%)	81	81
All	All	3558/5536 (64%)	3541 (100%)	17 (0%)	78	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	217	ILE
1	A	891	TYR
1	A	969	ARG
1	B	36	GLN
1	B	191	LEU
2	C	76	HIS

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Mol	Chain	Res	Type
2	C	87	LEU
2	D	76	HIS
2	D	212	HIS
3	E	283	LEU
1	G	79	ASP
1	G	147	ASP
1	G	1029	HIS
2	H	126	ASN
3	J	114	VAL
3	J	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	161	HIS
1	A	206	ASN
1	A	791	HIS
1	A	937	GLN
1	A	982	GLN
1	B	120	GLN
1	B	151	GLN
1	B	249	HIS
1	B	273	GLN
1	B	278	GLN
1	B	858	GLN
1	B	901	HIS
1	B	937	GLN
2	D	153	GLN
3	E	64	HIS
3	E	180	GLN
3	E	256	GLN
3	E	286	HIS
3	E	325	HIS
3	E	415	GLN
1	F	30	HIS
1	F	67	ASN
1	F	155	HIS
1	F	206	ASN
1	F	791	HIS
1	F	830	GLN
1	F	865	HIS

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Mol	Chain	Res	Type
1	F	937	GLN
1	F	982	GLN
1	G	120	GLN
1	G	151	GLN
1	G	273	GLN
1	G	278	GLN
1	G	791	HIS
1	G	858	GLN
1	G	937	GLN
2	H	218	ASN
3	J	184	HIS
3	J	325	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	G	1101	-	28,29,29	2.22	9 (32%)	43,45,45	1.80	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	F	1101	-	28,29,29	2.20	9 (32%)	43,45,45	1.79	8 (18%)
4	ADP	B	1101	-	28,29,29	2.22	9 (32%)	43,45,45	1.79	7 (16%)
4	ADP	A	1101	-	28,29,29	2.19	9 (32%)	43,45,45	1.79	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	G	1101	-	-	7/16/32/32	0/3/3/3
4	ADP	F	1101	-	-	6/16/32/32	0/3/3/3
4	ADP	B	1101	-	-	4/16/32/32	0/3/3/3
4	ADP	A	1101	-	-	7/16/32/32	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1101	ADP	PA-O3A	5.05	1.65	1.59
4	B	1101	ADP	PA-O3A	5.03	1.64	1.59
4	F	1101	ADP	PA-O3A	4.91	1.64	1.59
4	B	1101	ADP	C5-N7	4.80	1.47	1.39
4	A	1101	ADP	C5-N7	4.80	1.47	1.39
4	G	1101	ADP	C5-N7	4.80	1.47	1.39
4	F	1101	ADP	C5-N7	4.79	1.47	1.39
4	A	1101	ADP	PA-O3A	4.77	1.64	1.59
4	G	1101	ADP	C6-N6	4.44	1.45	1.34
4	B	1101	ADP	C6-N6	4.43	1.45	1.34
4	F	1101	ADP	C6-N6	4.43	1.45	1.34
4	A	1101	ADP	C6-N6	4.40	1.45	1.34
4	A	1101	ADP	C8-N9	-3.10	1.32	1.37
4	F	1101	ADP	C8-N9	-3.09	1.32	1.37
4	B	1101	ADP	C8-N9	-3.07	1.32	1.37
4	G	1101	ADP	C8-N9	-3.02	1.32	1.37
4	A	1101	ADP	O4'-C1'	2.56	1.47	1.42
4	B	1101	ADP	O4'-C1'	2.54	1.47	1.42
4	G	1101	ADP	O4'-C1'	2.53	1.47	1.42
4	F	1101	ADP	O4'-C1'	2.52	1.47	1.42
4	B	1101	ADP	C4-N9	-2.48	1.32	1.37
4	G	1101	ADP	C4-N9	-2.48	1.32	1.37
4	A	1101	ADP	C2'-C3'	-2.41	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1101	ADP	C2'-C3'	-2.39	1.46	1.53
4	F	1101	ADP	C2'-C3'	-2.39	1.46	1.53
4	B	1101	ADP	C2'-C3'	-2.36	1.47	1.53
4	F	1101	ADP	C4-N9	-2.36	1.32	1.37
4	A	1101	ADP	PB-O2B	-2.35	1.46	1.54
4	F	1101	ADP	PB-O2B	-2.34	1.46	1.54
4	F	1101	ADP	PB-O3B	-2.32	1.46	1.54
4	A	1101	ADP	PB-O3B	-2.31	1.46	1.54
4	A	1101	ADP	C4-N9	-2.30	1.32	1.37
4	B	1101	ADP	PB-O3B	-2.28	1.46	1.54
4	G	1101	ADP	PB-O3B	-2.28	1.46	1.54
4	G	1101	ADP	PB-O2B	-2.27	1.46	1.54
4	B	1101	ADP	PB-O2B	-2.26	1.46	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1101	ADP	C4-N9-C8	8.04	114.18	105.74
4	A	1101	ADP	C4-N9-C8	8.01	114.15	105.74
4	G	1101	ADP	C4-N9-C8	7.99	114.13	105.74
4	B	1101	ADP	C4-N9-C8	7.98	114.12	105.74
4	A	1101	ADP	O3B-PB-O3A	2.95	114.54	104.64
4	F	1101	ADP	O3B-PB-O3A	2.94	114.51	104.64
4	G	1101	ADP	O2B-PB-O3A	2.78	113.97	104.64
4	B	1101	ADP	O2B-PB-O3A	2.78	113.95	104.64
4	G	1101	ADP	O3B-PB-O3A	2.70	113.69	104.64
4	B	1101	ADP	O3B-PB-O3A	2.68	113.64	104.64
4	F	1101	ADP	O2B-PB-O3A	2.68	113.61	104.64
4	A	1101	ADP	O2B-PB-O3A	2.64	113.50	104.64
4	G	1101	ADP	C3'-C2'-C1'	2.58	106.34	101.46
4	A	1101	ADP	C1'-N9-C8	-2.55	121.45	127.09
4	F	1101	ADP	C1'-N9-C8	-2.49	121.57	127.09
4	B	1101	ADP	C3'-C2'-C1'	2.49	106.17	101.46
4	G	1101	ADP	O2A-PA-O1A	-2.45	101.04	112.44
4	B	1101	ADP	O2A-PA-O1A	-2.45	101.07	112.44
4	A	1101	ADP	C3'-C2'-C1'	2.38	105.96	101.46
4	A	1101	ADP	O2A-PA-O1A	-2.35	101.53	112.44
4	F	1101	ADP	O2A-PA-O1A	-2.34	101.54	112.44
4	F	1101	ADP	C3'-C2'-C1'	2.27	105.75	101.46
4	F	1101	ADP	C5-C4-N9	-2.25	103.36	105.81
4	A	1101	ADP	N3-C4-N9	2.25	131.00	127.17
4	F	1101	ADP	N3-C4-N9	2.21	130.93	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	ADP	C5-C4-N9	-2.20	103.42	105.81
4	G	1101	ADP	C2'-C3'-C4'	2.08	106.63	102.61
4	G	1101	ADP	C5-C4-N9	-2.07	103.56	105.81
4	B	1101	ADP	C5-C4-N9	-2.04	103.58	105.81
4	B	1101	ADP	C1'-N9-C8	-2.01	122.63	127.09
4	G	1101	ADP	C1'-N9-C8	-2.00	122.65	127.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	ADP	C5'-O5'-PA-O1A
4	A	1101	ADP	C5'-O5'-PA-O2A
4	A	1101	ADP	C5'-O5'-PA-O3A
4	B	1101	ADP	C5'-O5'-PA-O1A
4	B	1101	ADP	C5'-O5'-PA-O3A
4	F	1101	ADP	C5'-O5'-PA-O1A
4	F	1101	ADP	C5'-O5'-PA-O2A
4	F	1101	ADP	C5'-O5'-PA-O3A
4	G	1101	ADP	C5'-O5'-PA-O3A
4	A	1101	ADP	PA-O3A-PB-O1B
4	F	1101	ADP	PA-O3A-PB-O1B
4	A	1101	ADP	PB-O3A-PA-O2A
4	B	1101	ADP	PB-O3A-PA-O1A
4	F	1101	ADP	PB-O3A-PA-O2A
4	G	1101	ADP	PB-O3A-PA-O2A
4	G	1101	ADP	C5'-O5'-PA-O2A
4	B	1101	ADP	C4'-C5'-O5'-PA
4	G	1101	ADP	C4'-C5'-O5'-PA
4	G	1101	ADP	PA-O3A-PB-O2B
4	F	1101	ADP	PB-O3A-PA-O1A
4	G	1101	ADP	PB-O3A-PA-O1A
4	G	1101	ADP	O4'-C4'-C5'-O5'
4	A	1101	ADP	PB-O3A-PA-O1A
4	A	1101	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 10 short contacts:

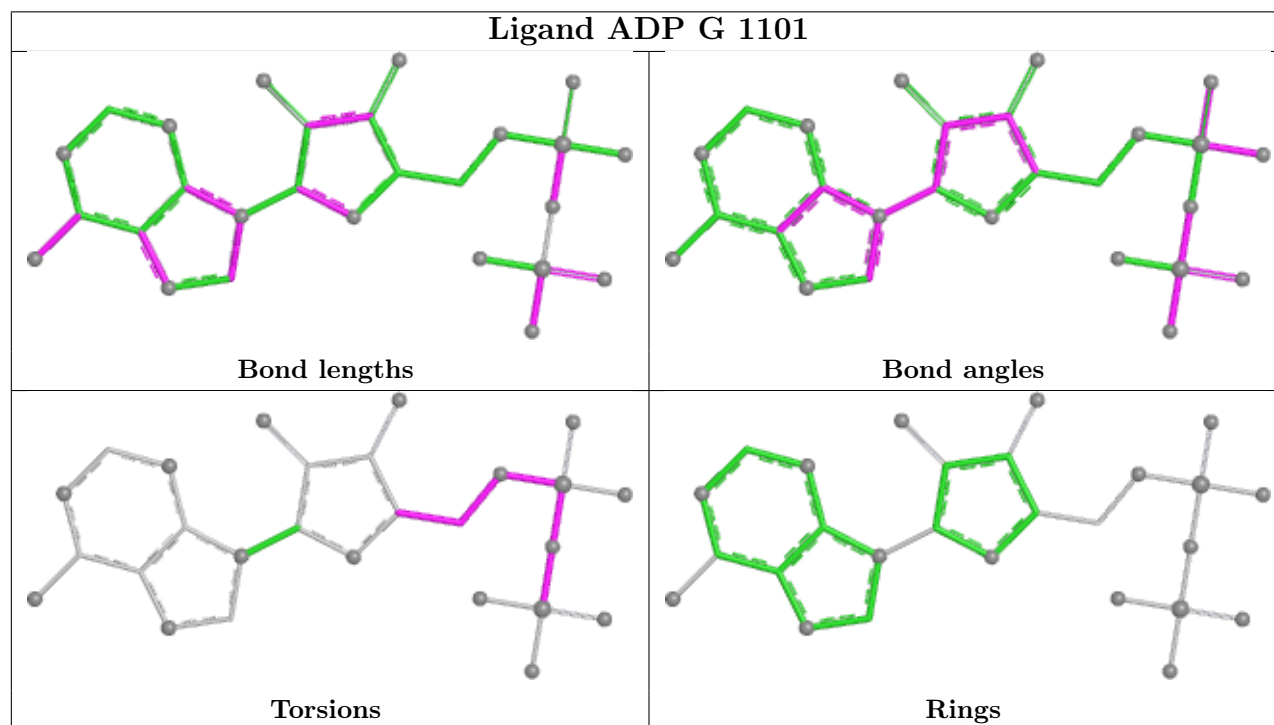
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1101	ADP	2	0

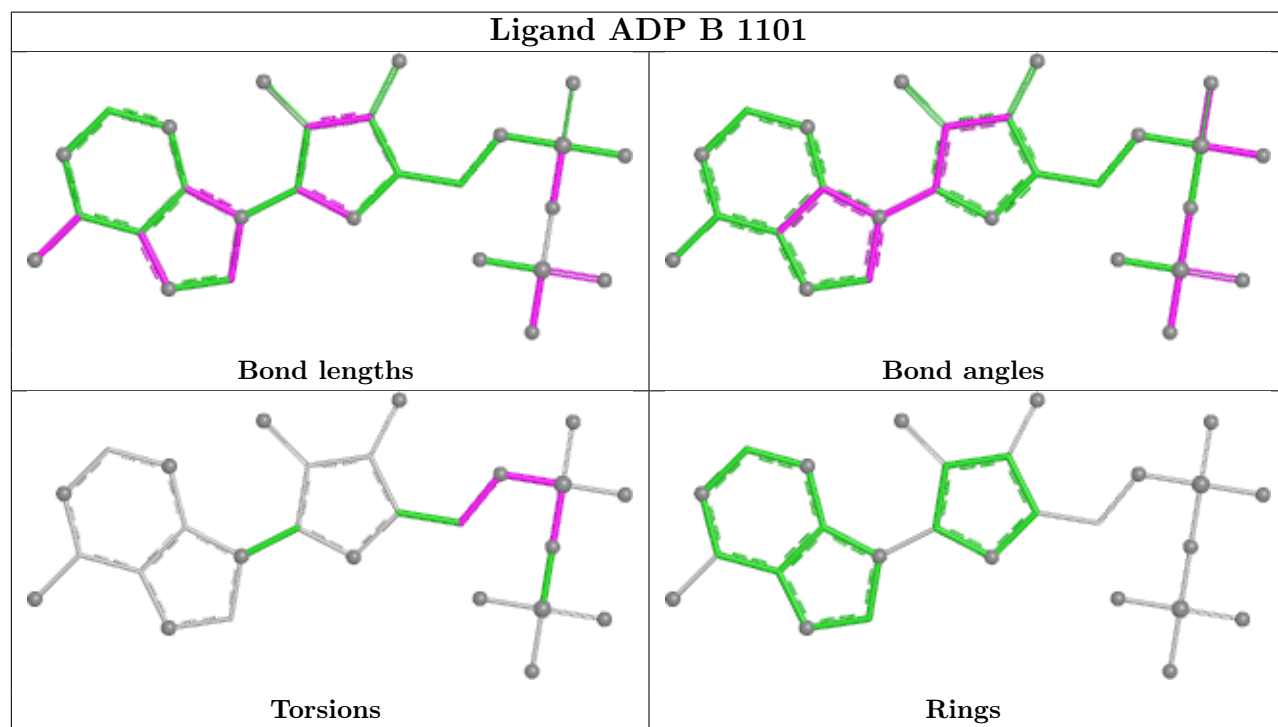
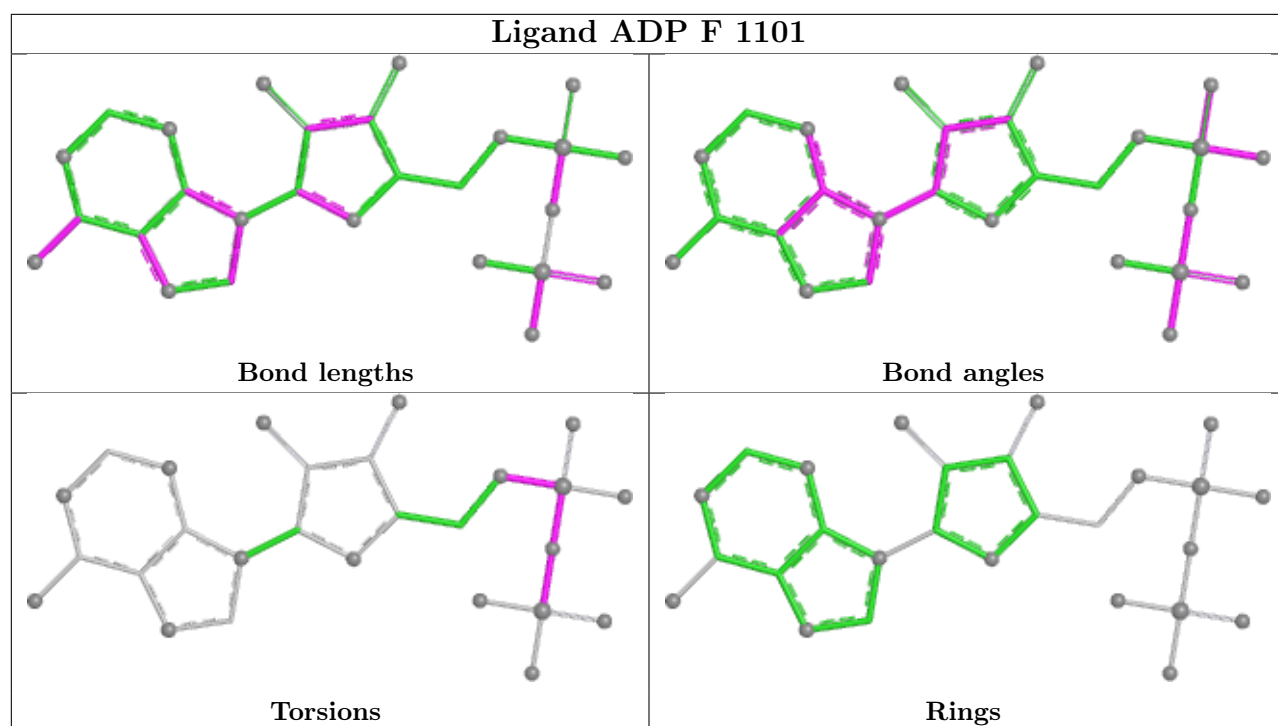
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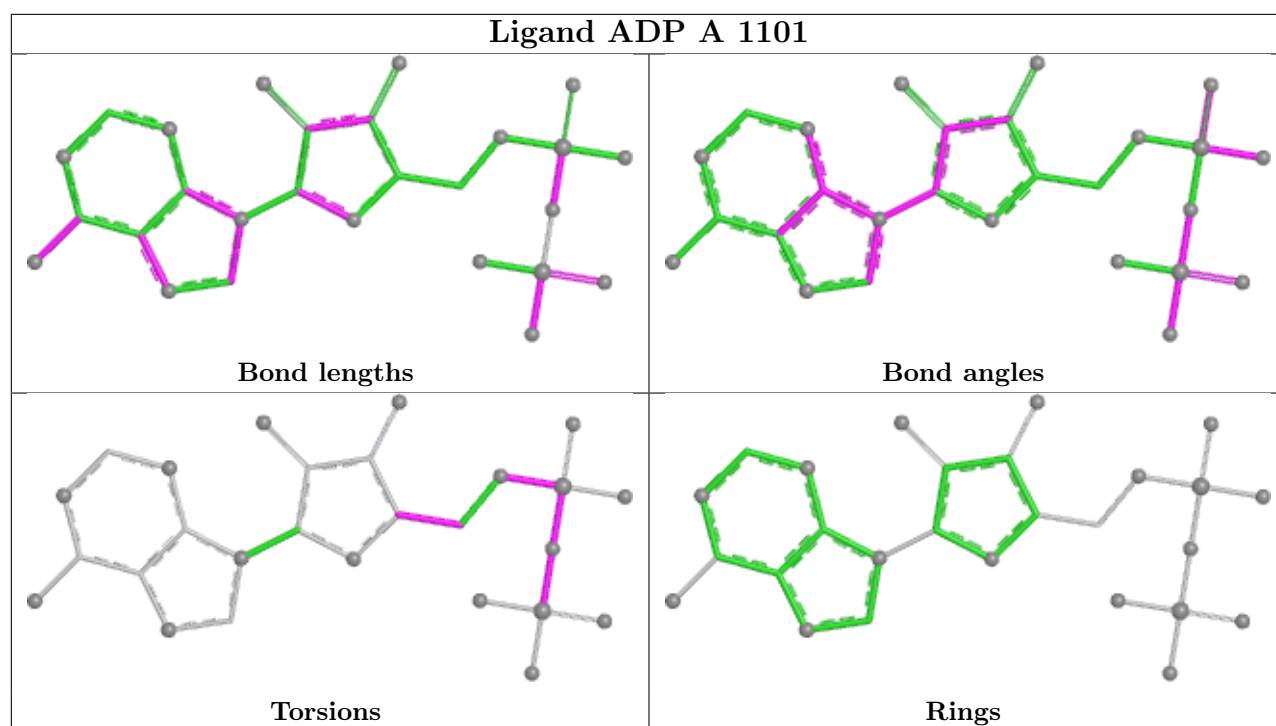
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1101	ADP	3	0
4	B	1101	ADP	4	0
4	A	1101	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

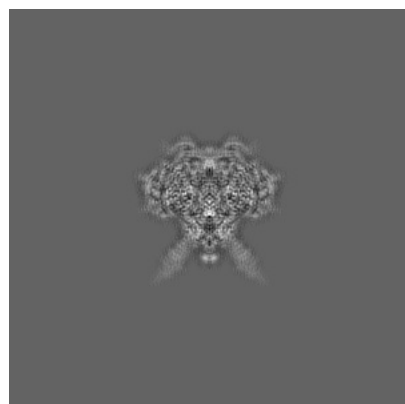
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16020. These allow visual inspection of the internal detail of the map and identification of artifacts.

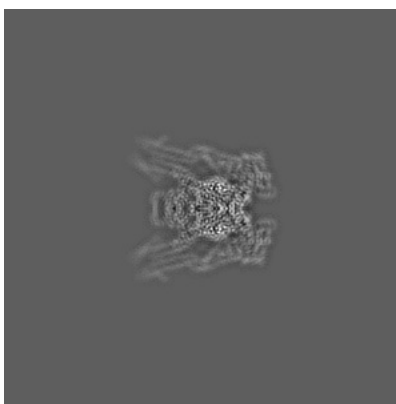
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

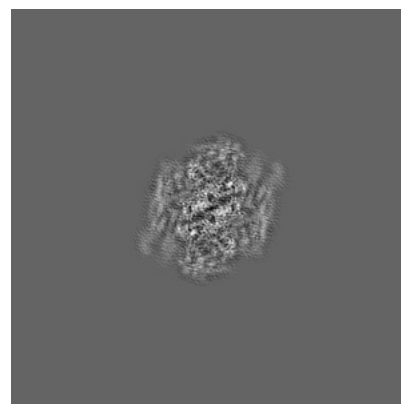
6.1.1 Primary map



X

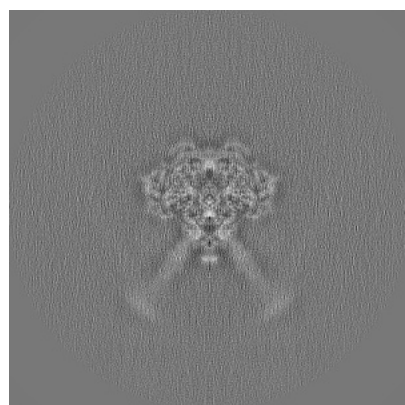


Y

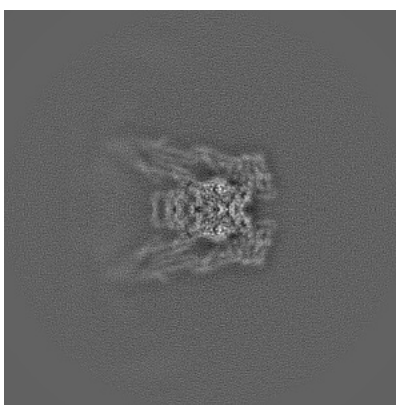


Z

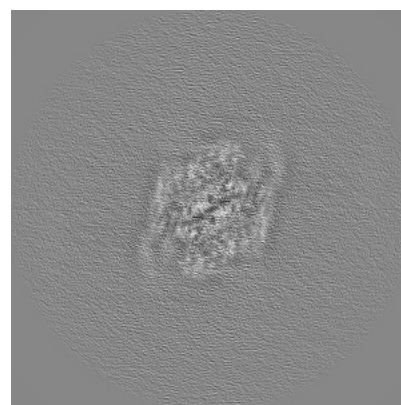
6.1.2 Raw map



X



Y

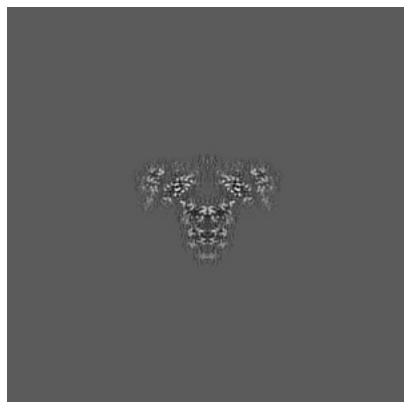


Z

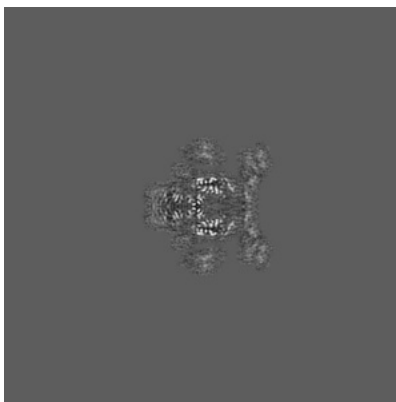
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

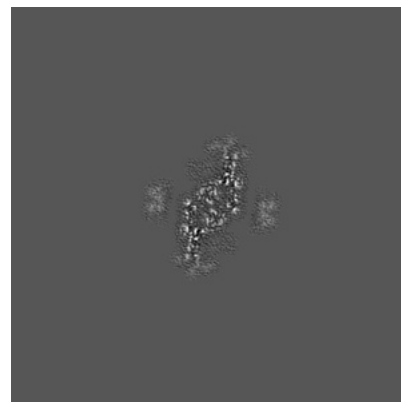
6.2.1 Primary map



X Index: 200

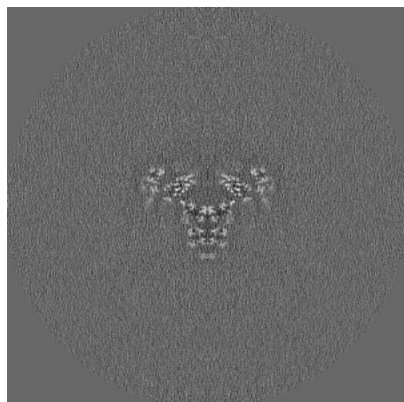


Y Index: 200

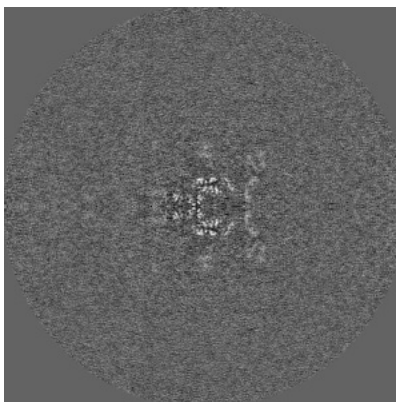


Z Index: 200

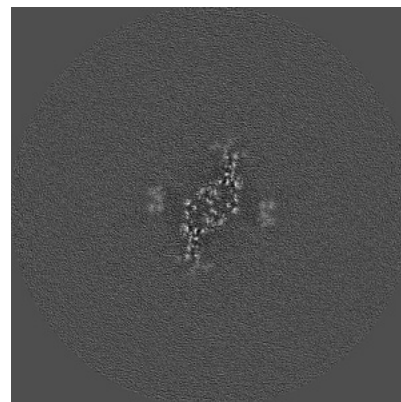
6.2.2 Raw map



X Index: 200



Y Index: 200

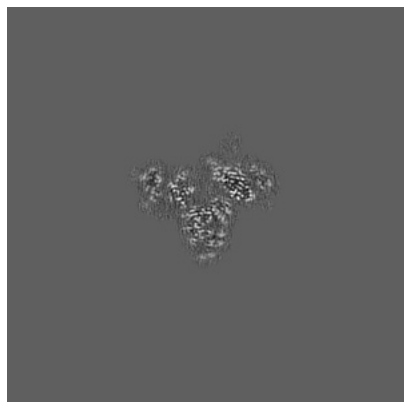


Z Index: 200

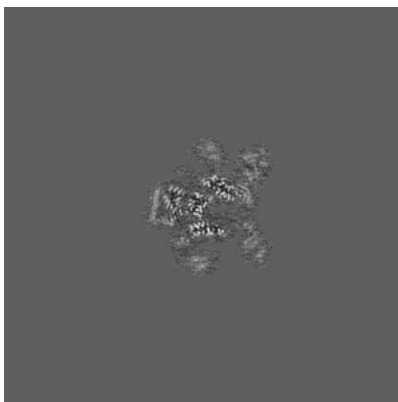
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

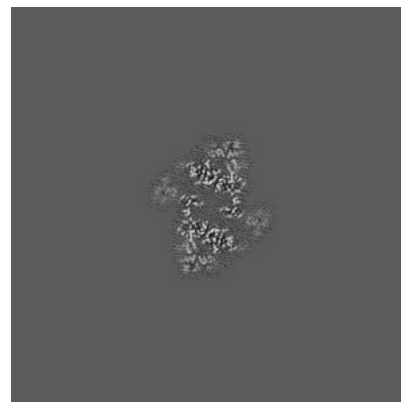
6.3.1 Primary map



X Index: 195

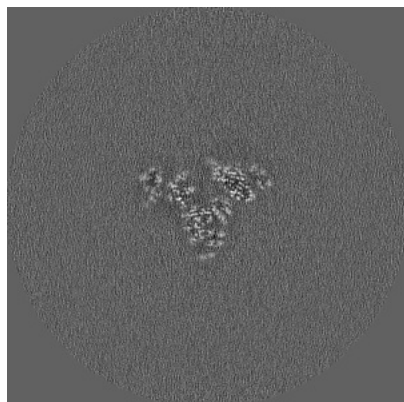


Y Index: 196

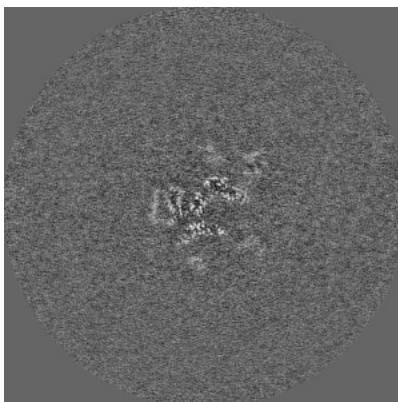


Z Index: 215

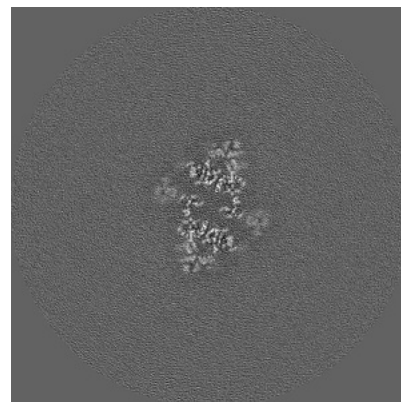
6.3.2 Raw map



X Index: 195



Y Index: 195

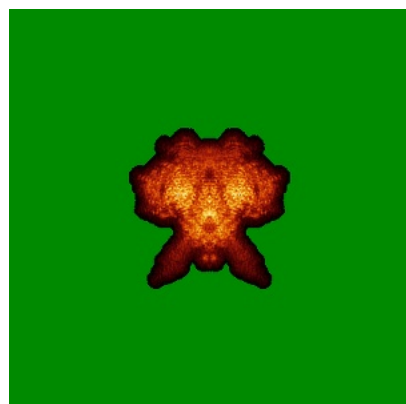


Z Index: 215

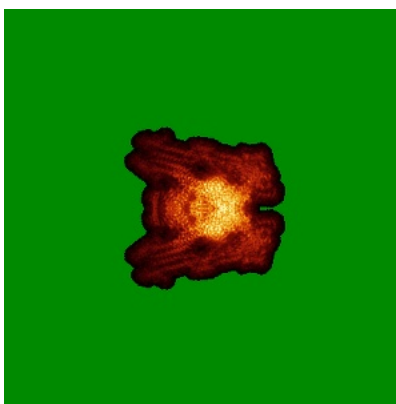
The images above show the largest variance slices of the map in three orthogonal directions.

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

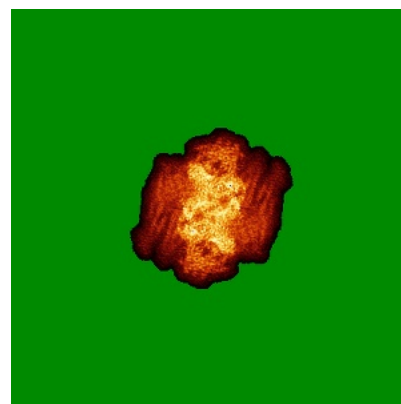
6.4.1 Primary map



X

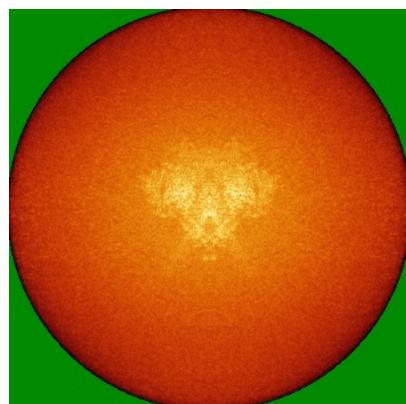


Y

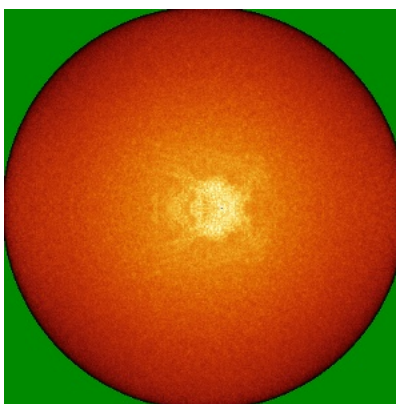


Z

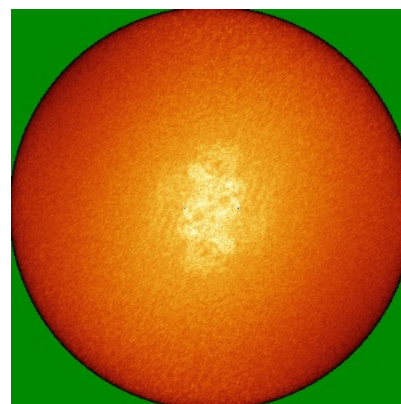
6.4.2 Raw map



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.

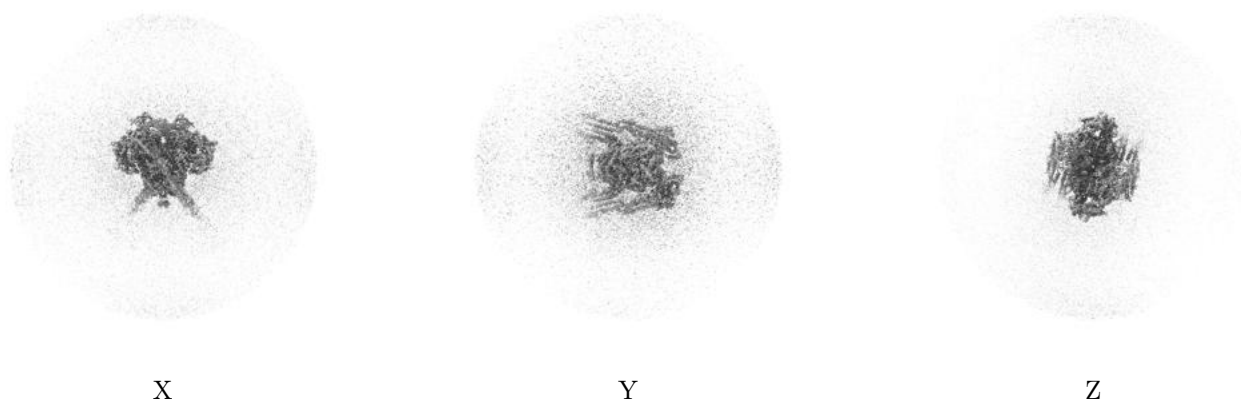
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00296. 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.

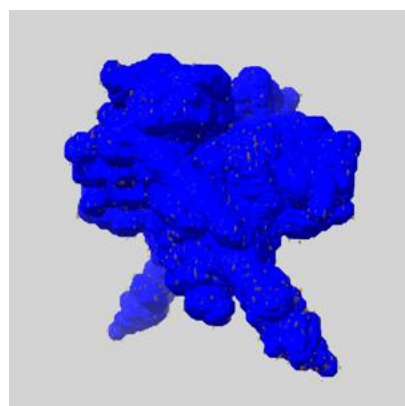
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

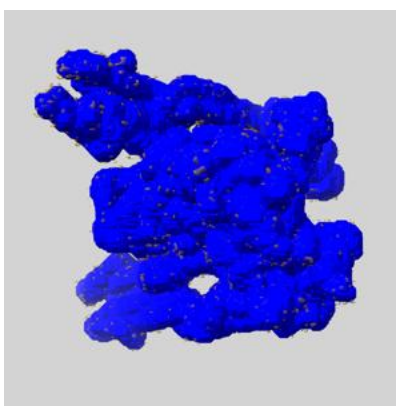
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

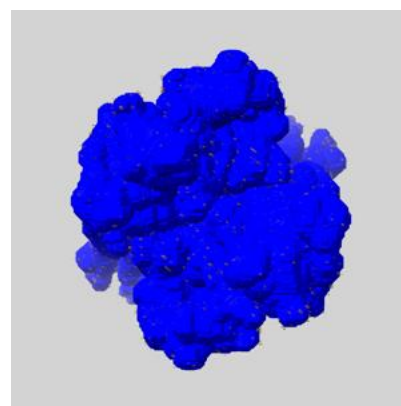
6.6.1 emd_16020_msk_1.map [i](#)



X



Y

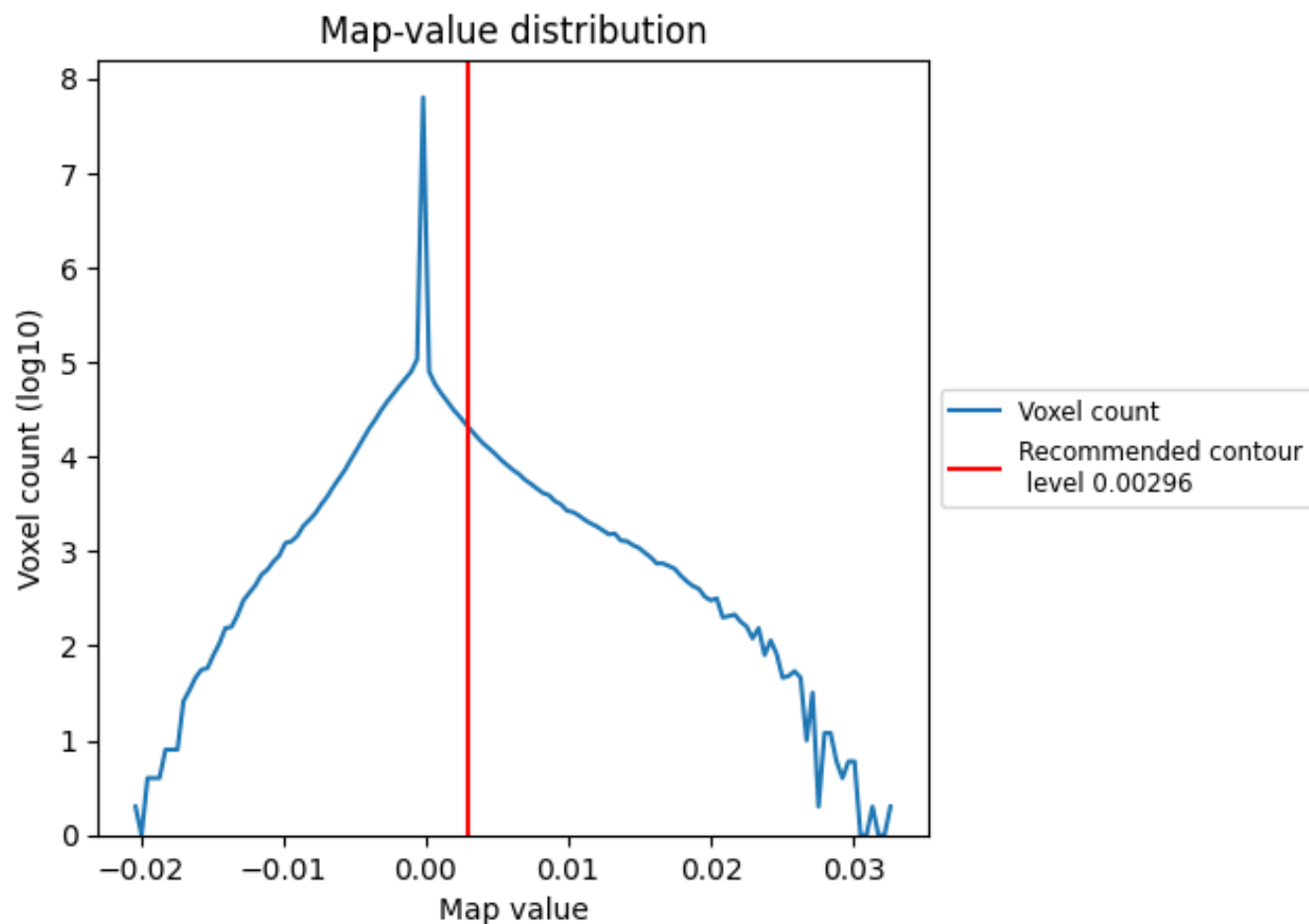


Z

7 Map analysis [i](#)

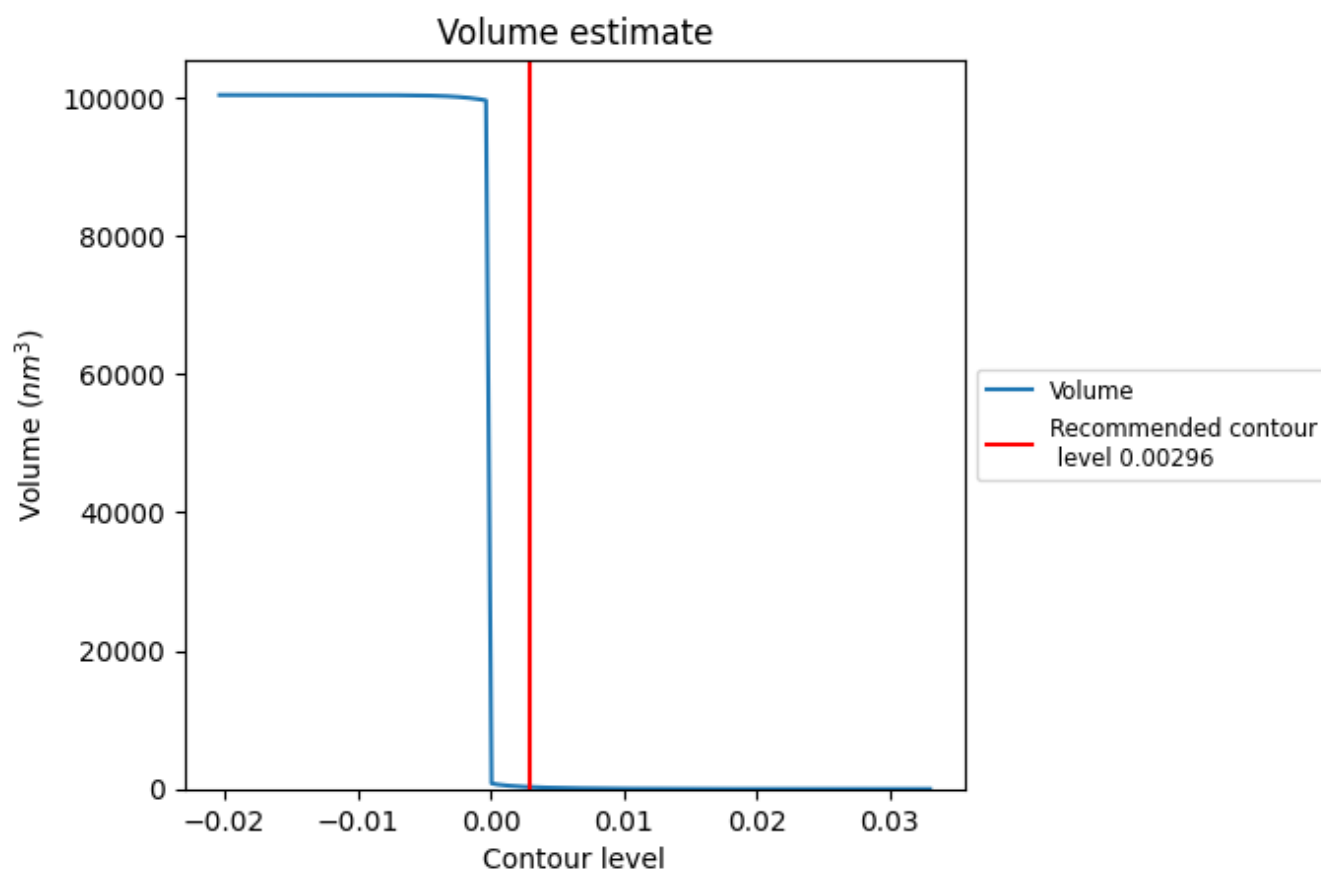
This section contains the results of statistical analysis of the map.

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.

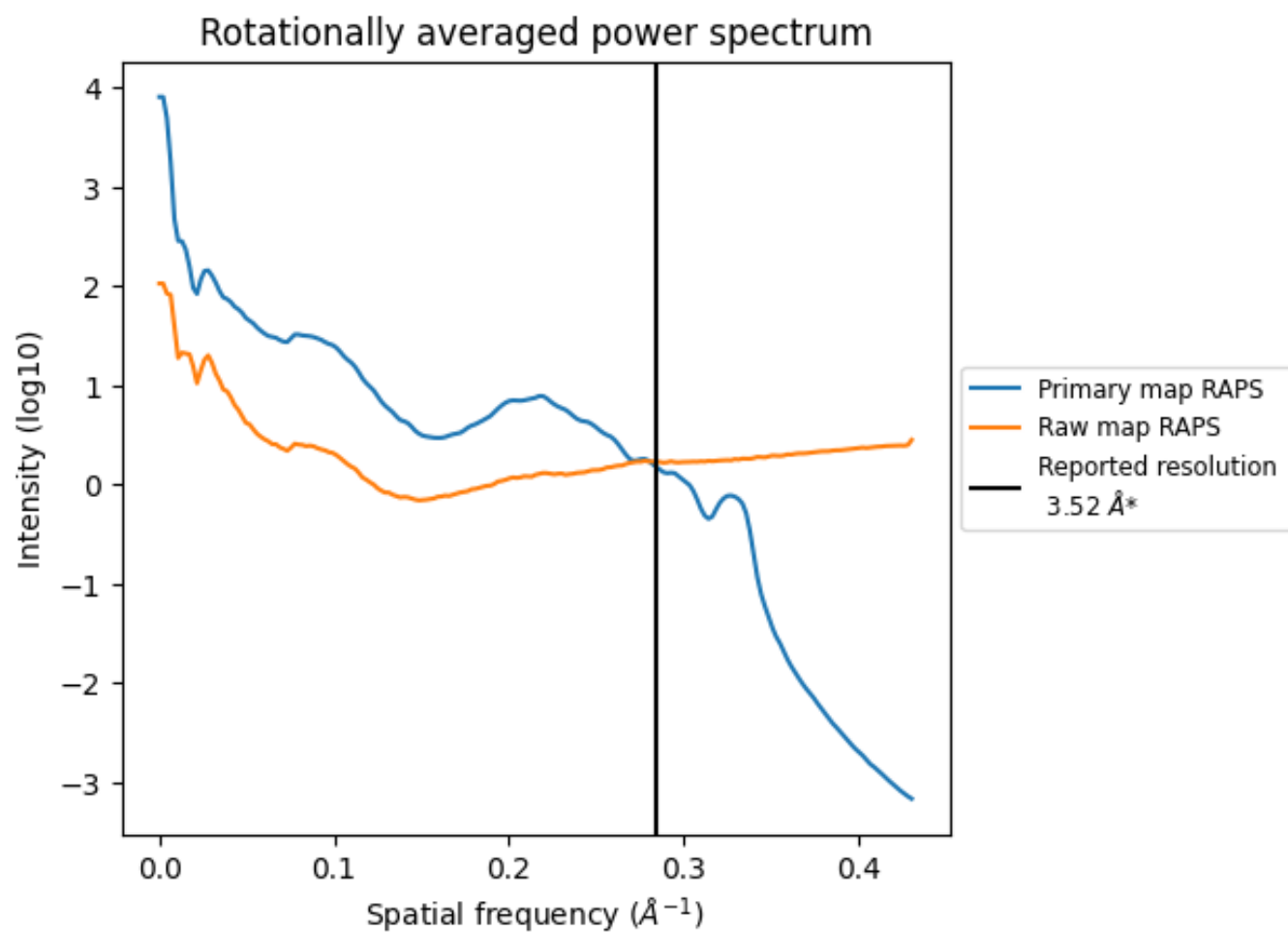
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm³; this corresponds to an approximate mass of 251 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 ⓘ

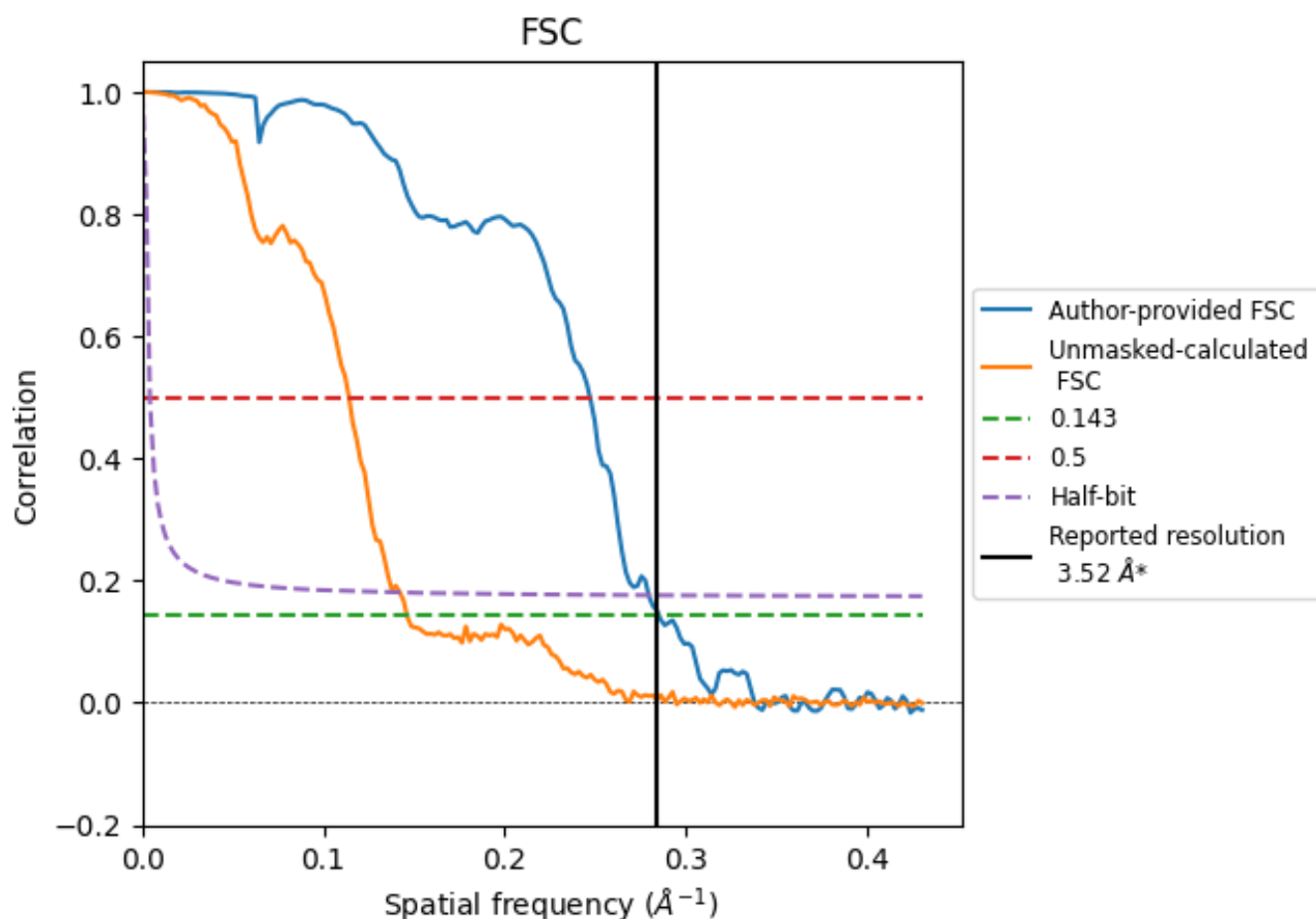


*Reported resolution corresponds to spatial frequency of 0.284 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.284 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

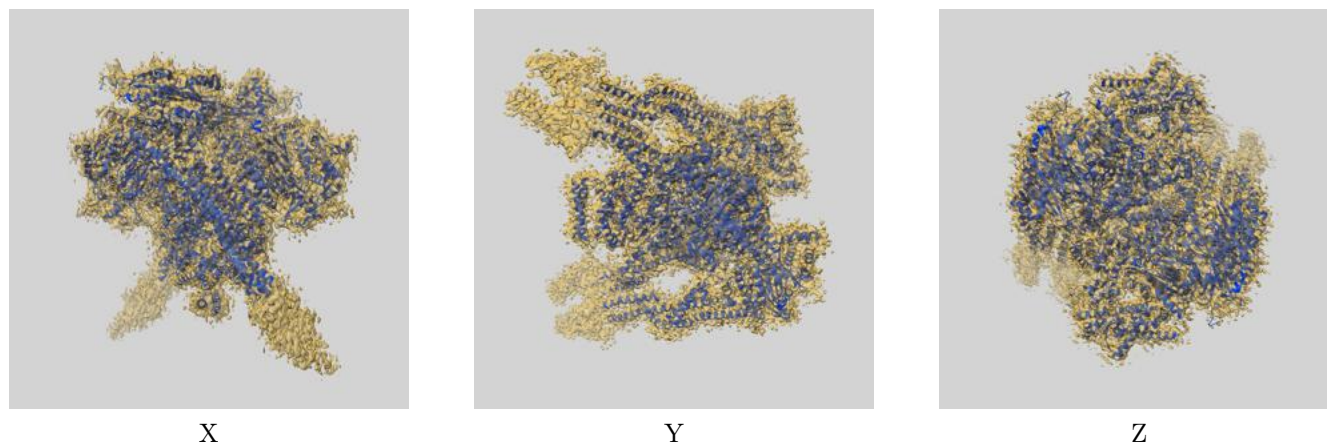
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.51	4.05	3.58
Unmasked-calculated*	6.84	8.76	7.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 3.52 by more than 10 %

9 Map-model fit [i](#)

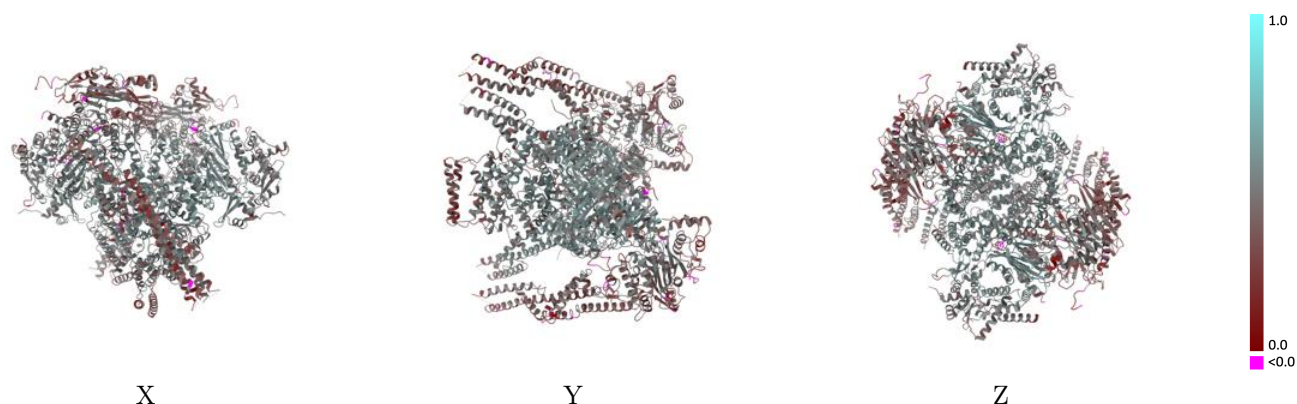
This section contains information regarding the fit between EMDB map EMD-16020 and PDB model 8BFN. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



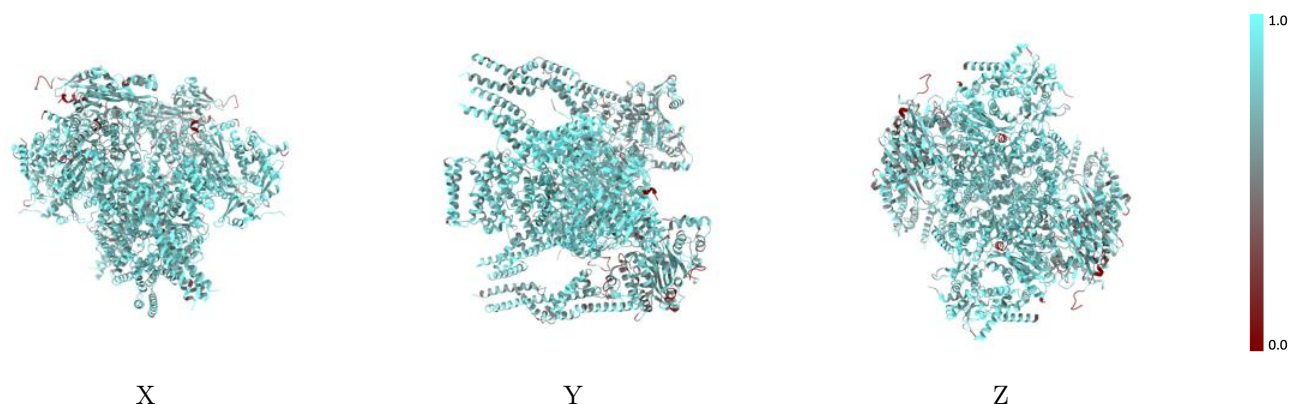
The images above show the 3D surface view of the map at the recommended contour level 0.00296 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



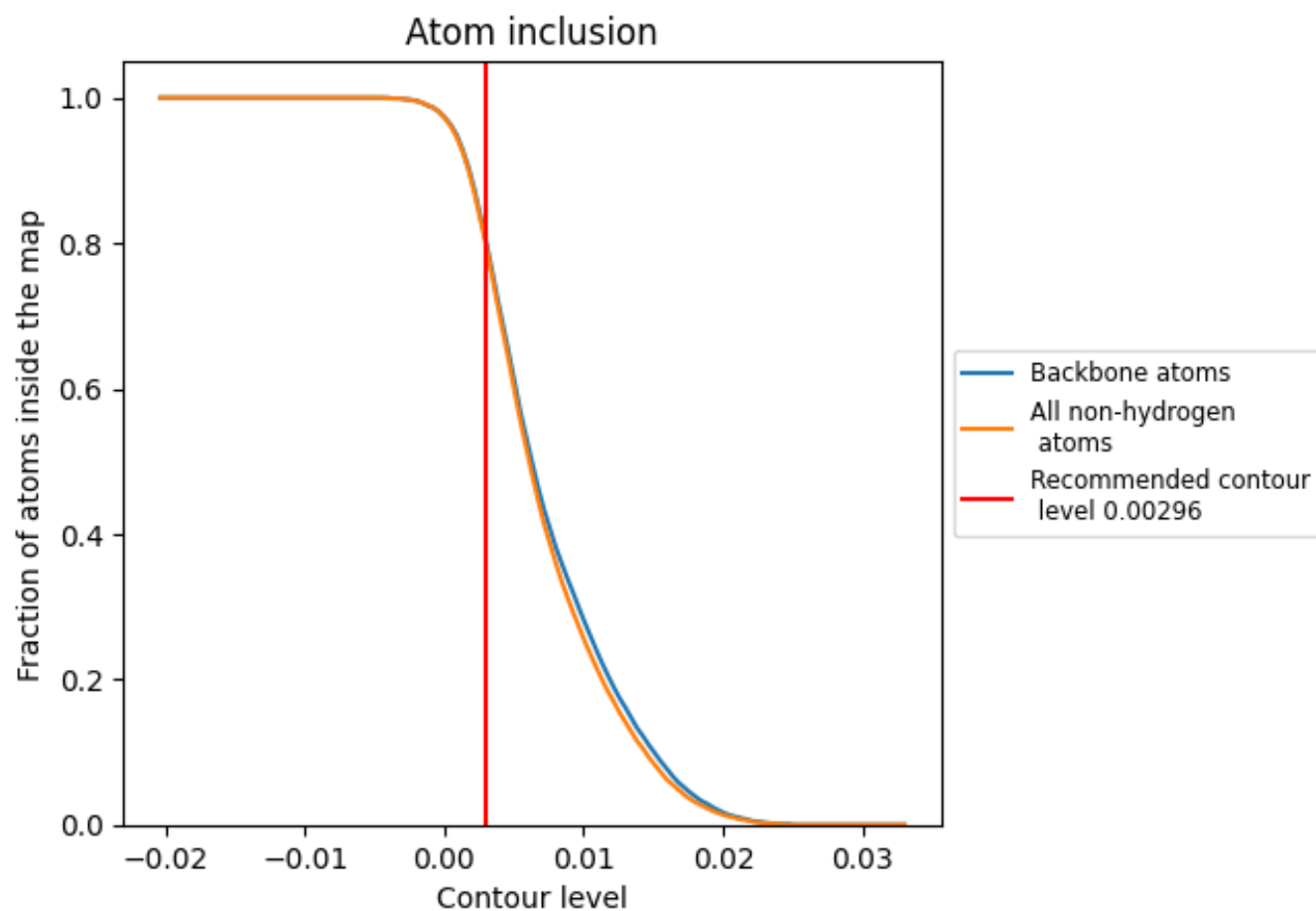
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00296).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.00296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.4520
A	0.8470	0.5050
B	0.7020	0.3640
C	0.8910	0.5210
D	0.8390	0.4640
E	0.8230	0.4540
F	0.8530	0.5090
G	0.7020	0.3670
H	0.8950	0.5240
I	0.8460	0.4680
J	0.8270	0.4580

1.0

0.0

<0.0