Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 03:36 pm GMT

PDB ID	:	8BFN
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)

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

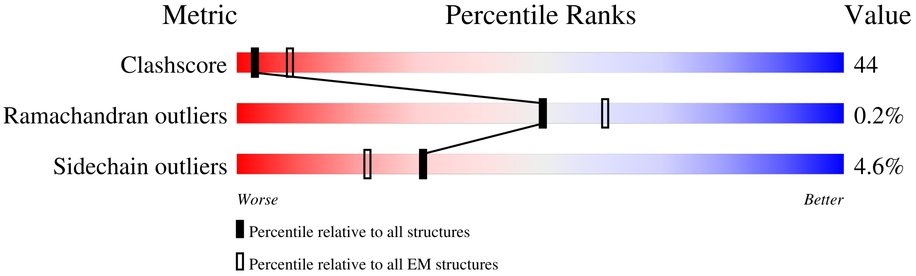
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

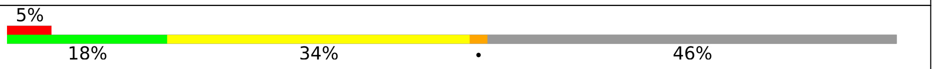
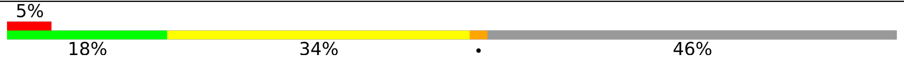
The reported resolution of this entry is 3.52 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1096	
1	B	1096	
1	F	1096	
1	G	1096	
2	C	250	
2	D	250	
2	H	250	
2	I	250	

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Mol	Chain	Length	Quality of chain
3	E	554	
3	J	554	

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 4735	C 2955	N 869	O 899	S 12	0	0
1	B	597	Total 4735	C 2955	N 869	O 899	S 12	0	0
1	F	597	Total 4735	C 2955	N 869	O 899	S 12	0	0
1	G	597	Total 4735	C 2955	N 869	O 899	S 12	0	0

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 1566	C 991	N 280	O 295	0	0
2	D	195	Total 1566	C 991	N 280	O 295	0	0
2	H	195	Total 1566	C 991	N 280	O 295	0	0
2	I	195	Total 1566	C 991	N 280	O 295	0	0

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 4044	C 2512	N 752	O 772	S 8	0	0
3	J	498	Total 4044	C 2512	N 752	O 772	S 8	0	0

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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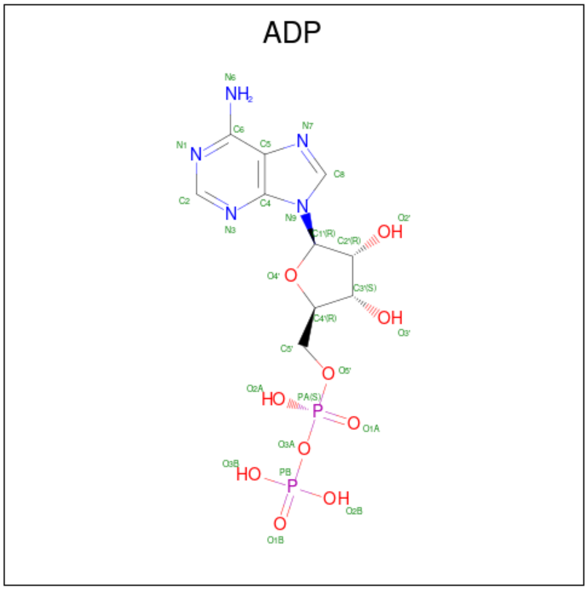
Chain	Residue	Modelled	Actual	Comment	Reference
J	-23	GLY	-	expression tag	UNP A0A4V3QHV5
J	-22	SER	-	expression tag	UNP A0A4V3QHV5
J	-21	GLY	-	expression tag	UNP A0A4V3QHV5
J	-20	GLY	-	expression tag	UNP A0A4V3QHV5
J	-19	GLY	-	expression tag	UNP A0A4V3QHV5
J	-18	SER	-	expression tag	UNP A0A4V3QHV5
J	-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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



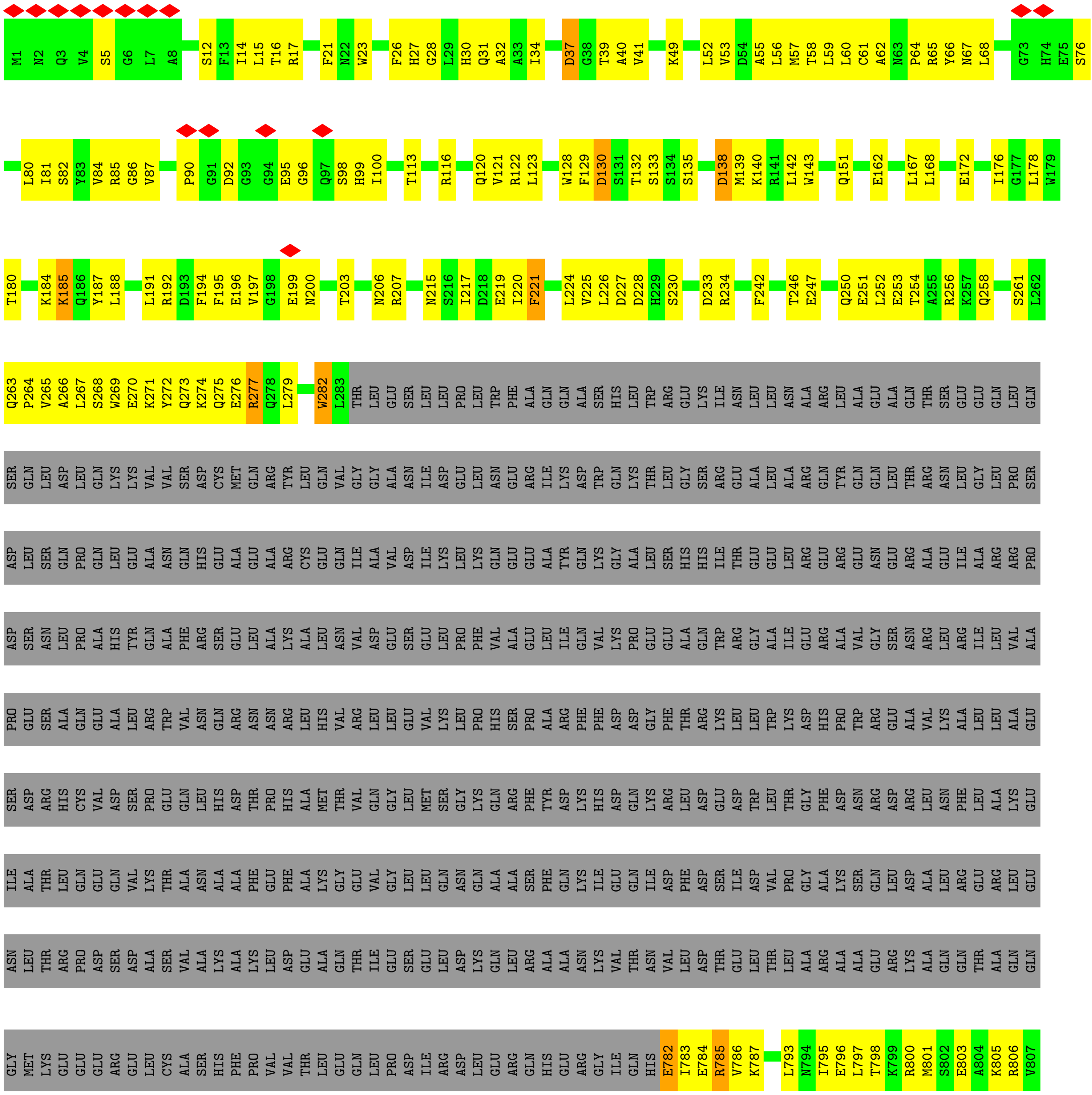
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C H N O P 39 10 12 5 10 2	0
4	B	1	Total C H N O P 39 10 12 5 10 2	0
4	F	1	Total C H N O P 39 10 12 5 10 2	0
4	G	1	Total C H N O P 39 10 12 5 10 2	0

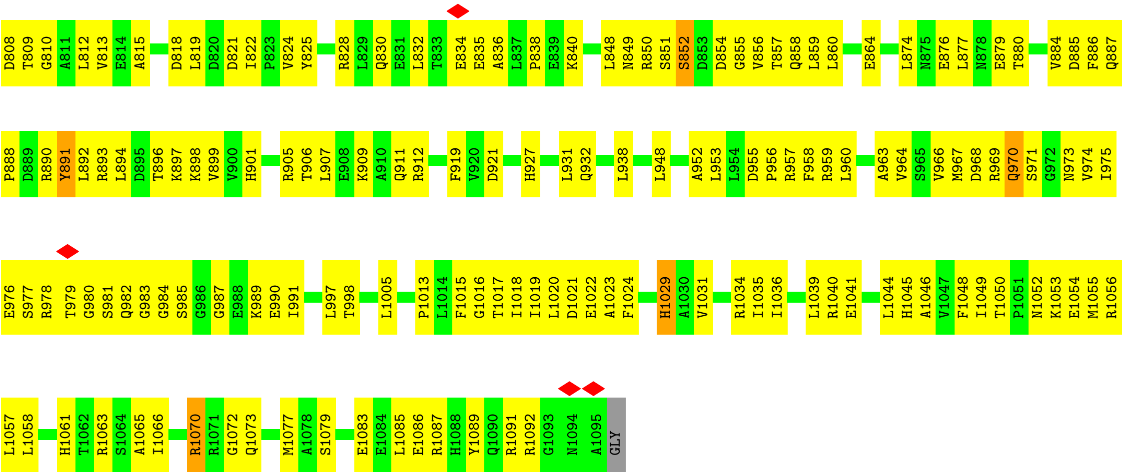
3 Residue-property plots ⓘ

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

- Molecule 1: JetC

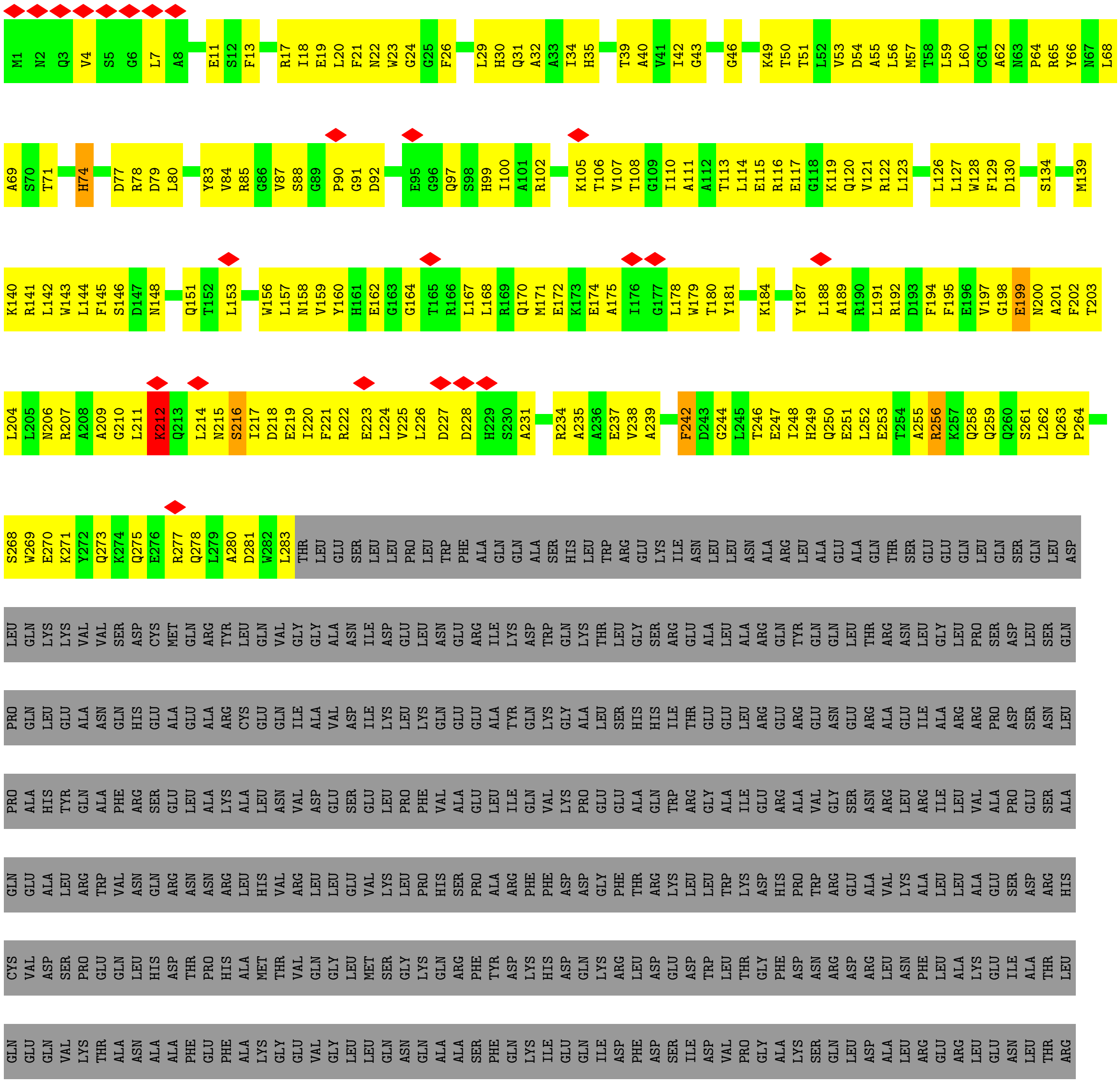
Chain A:

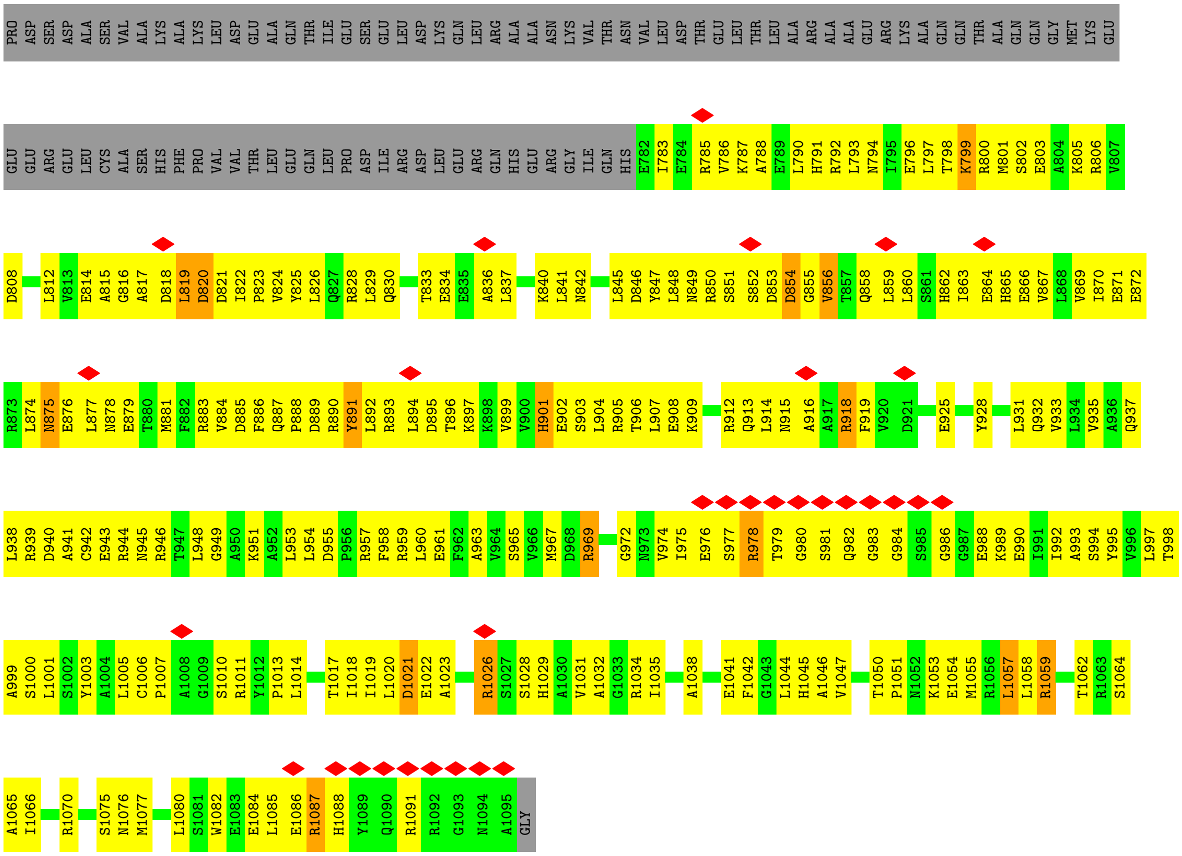




- Molecule 1: JetC

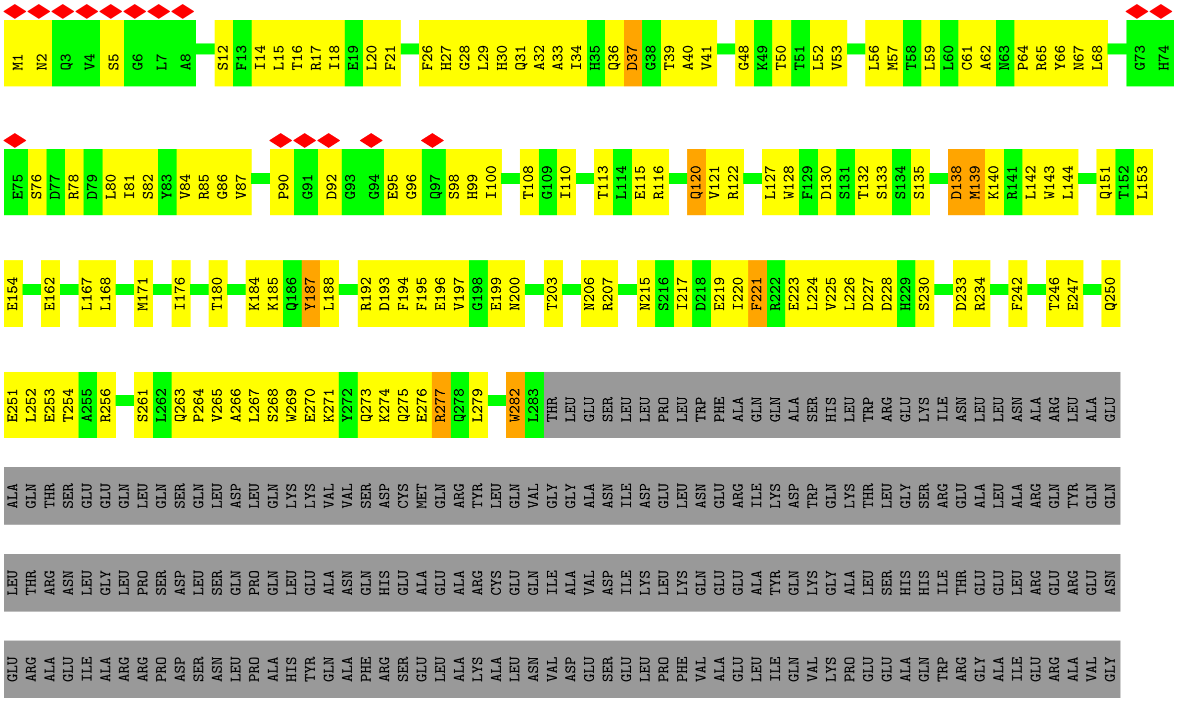
Chain B:

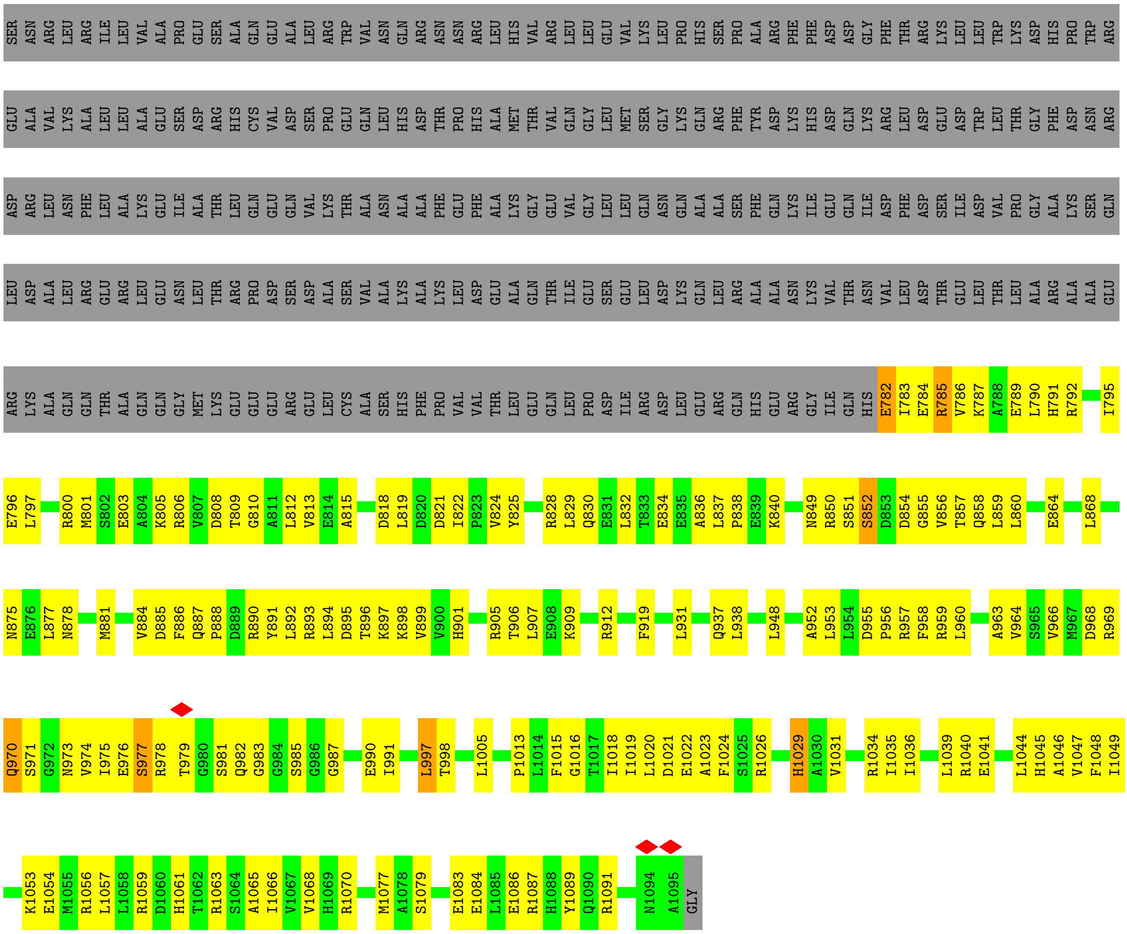




- Molecule 1: JetC

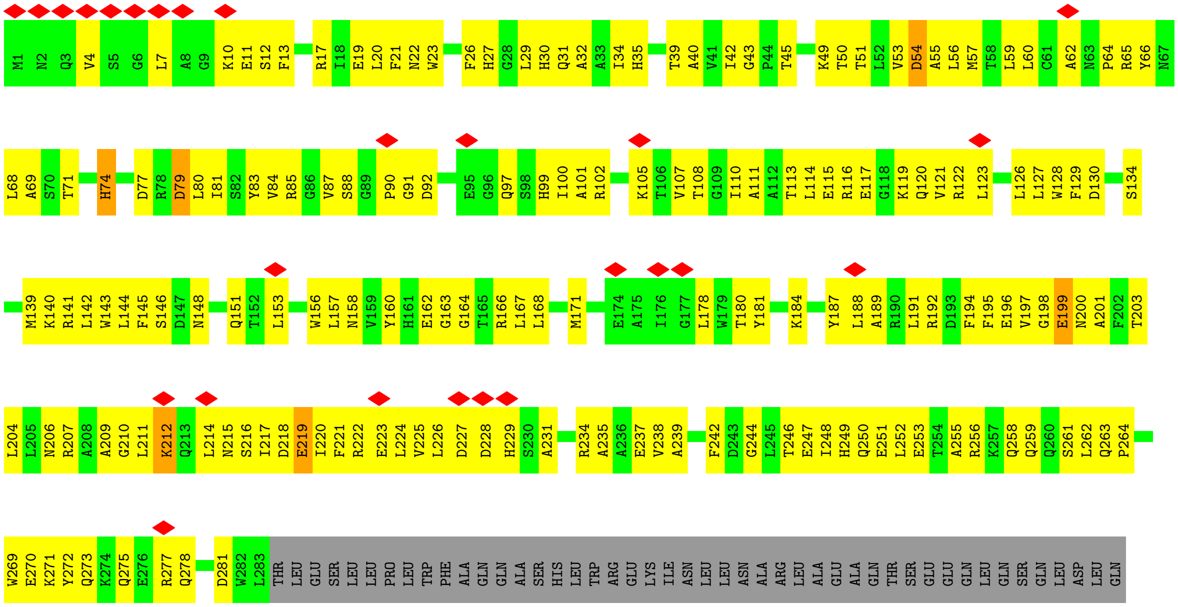
Chain F:

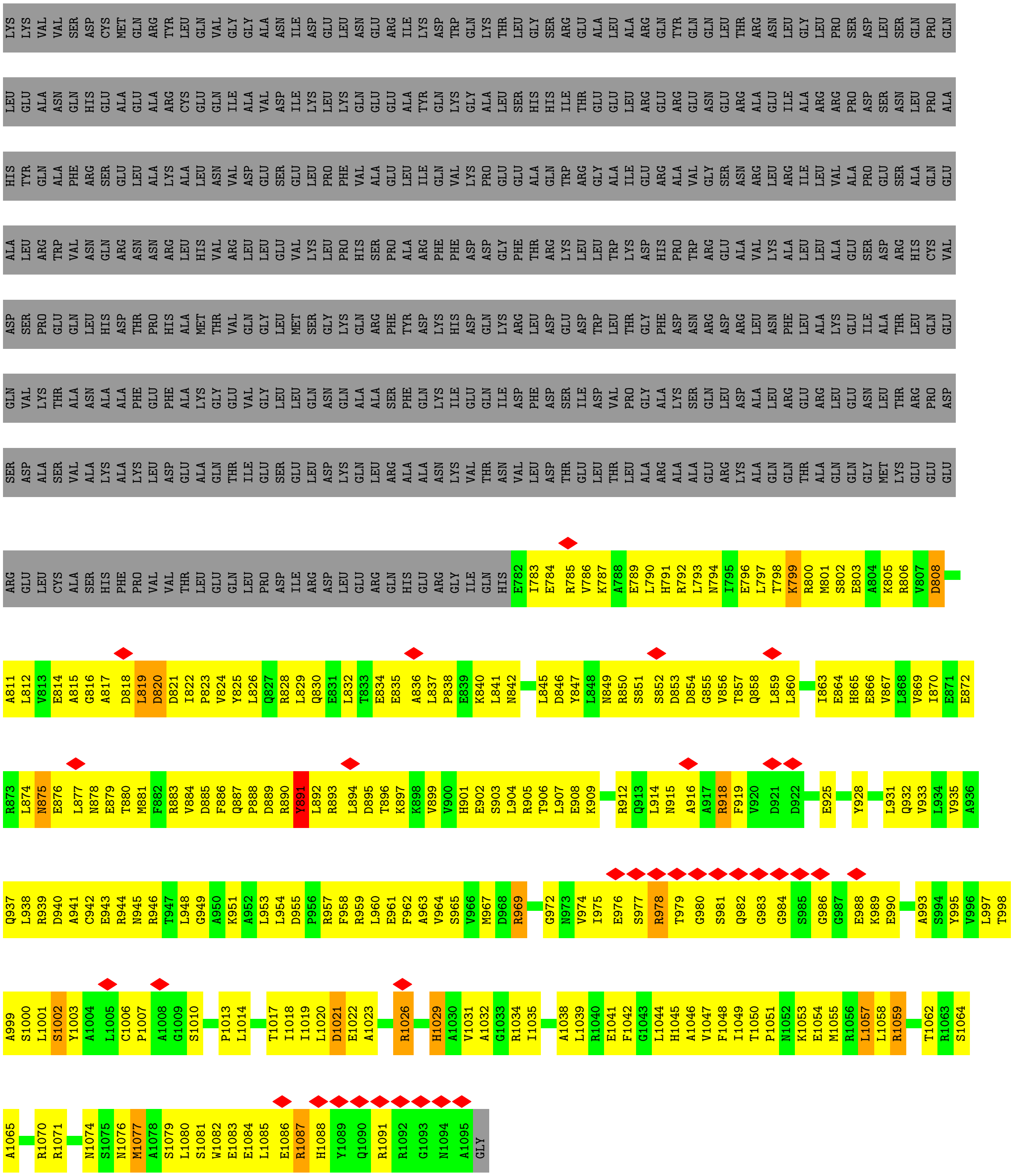




- Molecule 1: JetC

Chain G:





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

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

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

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

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

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

SER ASP ALA SER VAL ALA LYS ALA LYS LEU ASP GLU ALA GLN THR ILE GLU SER GLU LEU ASP LYS GLN LEU ARG ALA ALA ASN LYS VAL THR ASN VAL LEU ASP THR GLU LEU THR LEU ALA ARG ALA ALA GLU ARG LYS ALA GLN GLN THR ALA GLN GLN GLY MET LYS GLU GLU GLU

ARG GLU LEU CYS ALA SER HIS PHE PRO VAL VAL THR LEU GLN GLN LEU PRO ASP ILE ARG ASP LEU GLU ARG GLN HIS GLU ARG GLY ILE GLN HIS E782 I783 E784 R785 V786 K787 A788 E789 L790 H791 R792 L793 N794 I795 E796 L797 T798 K799 R800 M801 S802 E803 A804 K805 R806 V807 D808

A811 L812 V813 E814 A815 G816 A817 D818 L819 D820 D821 I822 P823 V824 Y825 L826 Q827 R828 L829 Q830 E831 L832 T833 E834 E835 A836 L837 P838 E839 K840 L841 N842 L845 D846 Y847 L848 N849 R850 S851 S852 D853 D854 G855 V856 T857 Q858 L859 L860 I863 E864 H865 E866 V867 L868 V869 I870 E871 E872

R873 L874 N875 E876 L877 N878 E879 T880 M881 F882 R883 V884 D885 F886 Q887 P888 D889 R890 Y891 L892 R893 L894 D895 T896 K897 K898 V899 V900 H901 E902 S903 L904 R905 T906 L907 E908 K909 R912 Q913 L914 N915 A916 A917 R918 F919 V920 D921 D922 E925 Y928 L931 Q932 V933 L934 V935 A936

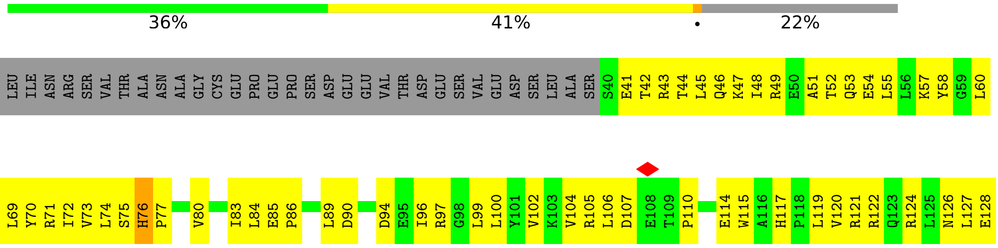
Q937 L938 R939 D940 A941 C942 E943 R944 N945 R946 T947 L948 G949 A950 K951 A952 L953 L954 D955 P956 R957 F958 R959 L960 E961 F962 A963 V964 S965 V966 M967 D968 R969 G972 N973 V974 I975 E976 S977 R978 T979 G980 S981 Q982 G983 G984 S985 G986 G987 E988 K989 E990 A993 S994 Y995 V996 L997 T998

A999 S1000 L1001 S1002 Y1003 A1004 L1005 C1006 P1007 A1008 G1009 S1010 P1013 L1014 T1017 I1018 I1019 L1020 D1021 E1022 A1023 R1026 H1029 A1030 V1031 A1032 G1033 R1034 I1035 A1038 L1039 R1040 E1041 F1042 G1043 L1044 H1045 A1046 V1047 F1048 I1049 T1050 P1051 N1052 K1053 E1054 M1055 R1056 L1057 L1058 R1059 T1062 R1063 S1064

A1065 R1070 R1071 N1074 S1075 N1076 M1077 A1078 S1079 L1080 S1081 W1082 E1083 E1084 L1085 E1086 R1087 H1088 Y1089 Q1090 R1091 R1092 G1093 N1094 A1095 GLY

- Molecule 2: JetB

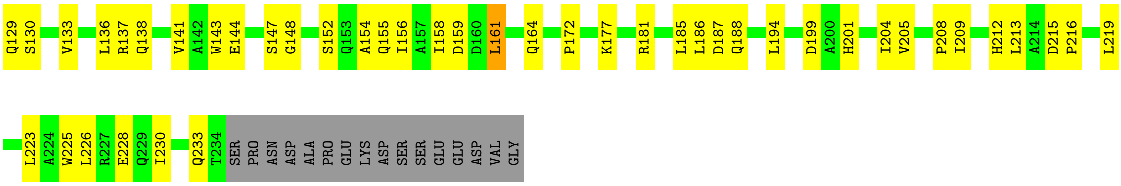
Chain C:



36% 41% • 22%

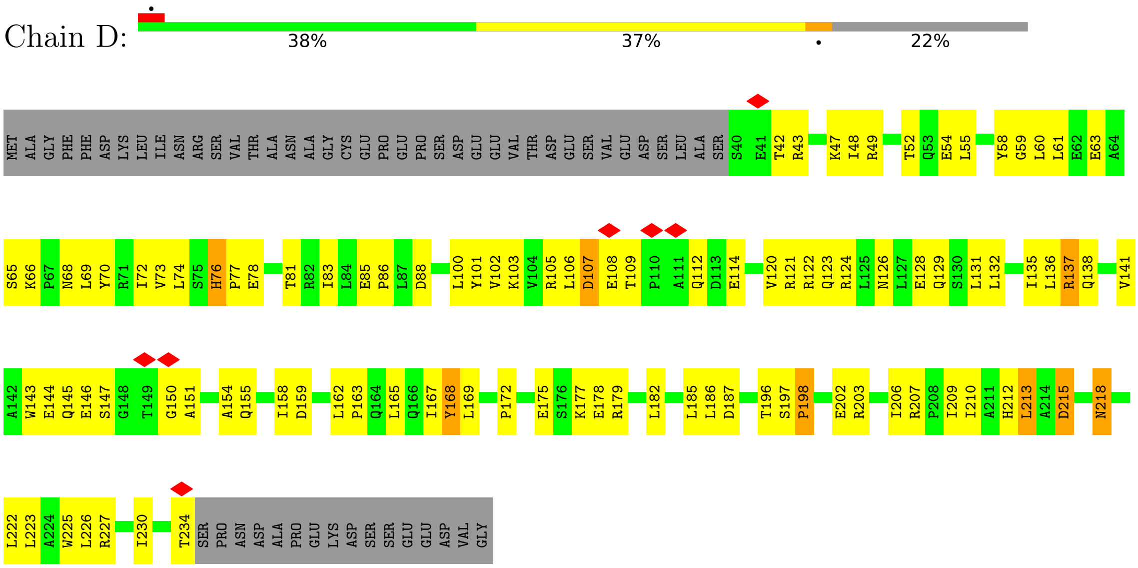
MET ALA GLY PHE PHE ASP LYS LEU ILE ASN ARG SER VAL THR ALA ASN ALA GLY CYS GLU PRO GLU PRO SER ASP GLU GLU VAL THR ASP GLU SER VAL GLU ASP SER LEU ALA SER S40 E41 T42 R43 T44 L45 Q46 K47 I48 R49 E50 A51 T52 Q53 E54 L55 L56 K57 Y58 G59 L60

L61 E62 E63 K66 P67 N68 L69 Y70 R71 I72 V73 L74 S75 H76 P77 V80 I83 L84 E85 P86 L89 D90 D94 E95 I96 R97 G98 L99 L100 Y101 V102 K103 V104 R105 L106 D107 E108 T109 P110 E114 W115 A116 H117 P118 L119 V120 R121 R122 Q123 R124 L125 N126 L127 E128



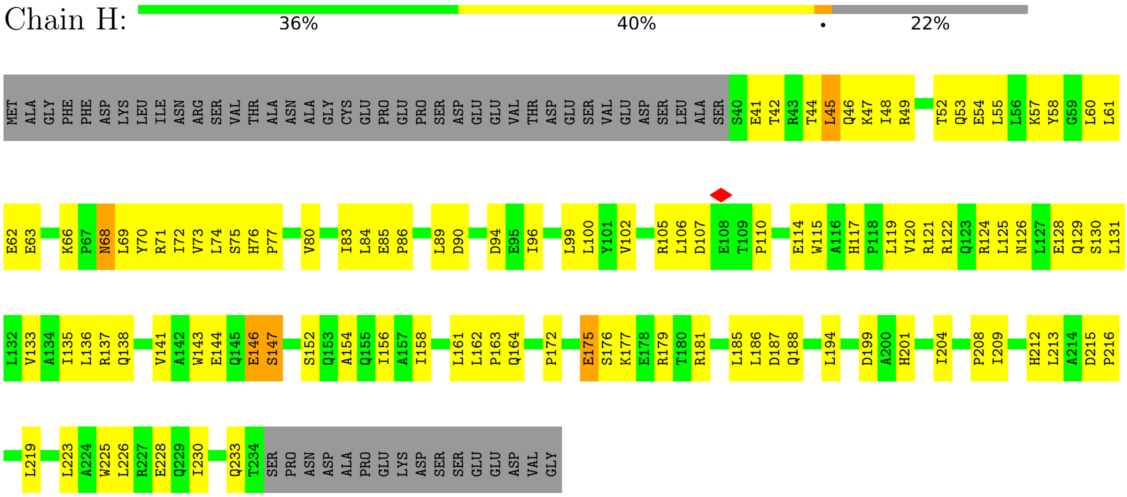
- Molecule 2: JetB

Chain D:



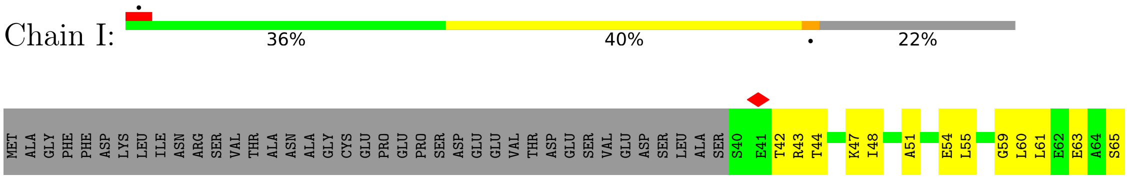
- Molecule 2: JetB

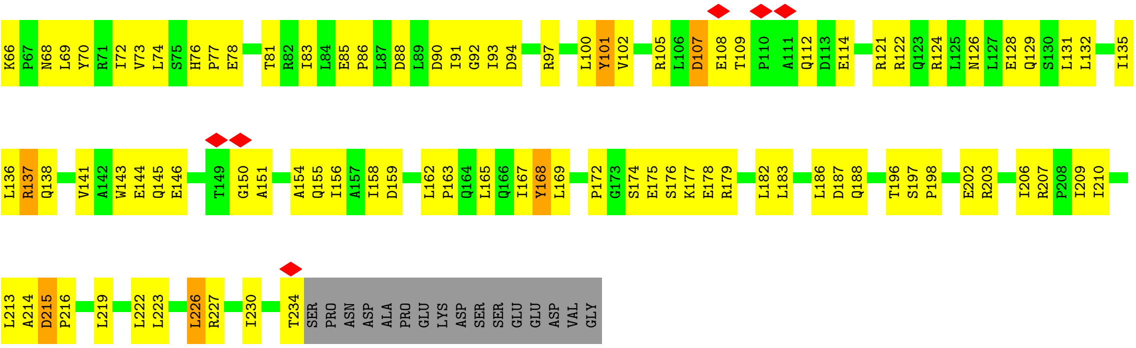
Chain H:



- Molecule 2: JetB

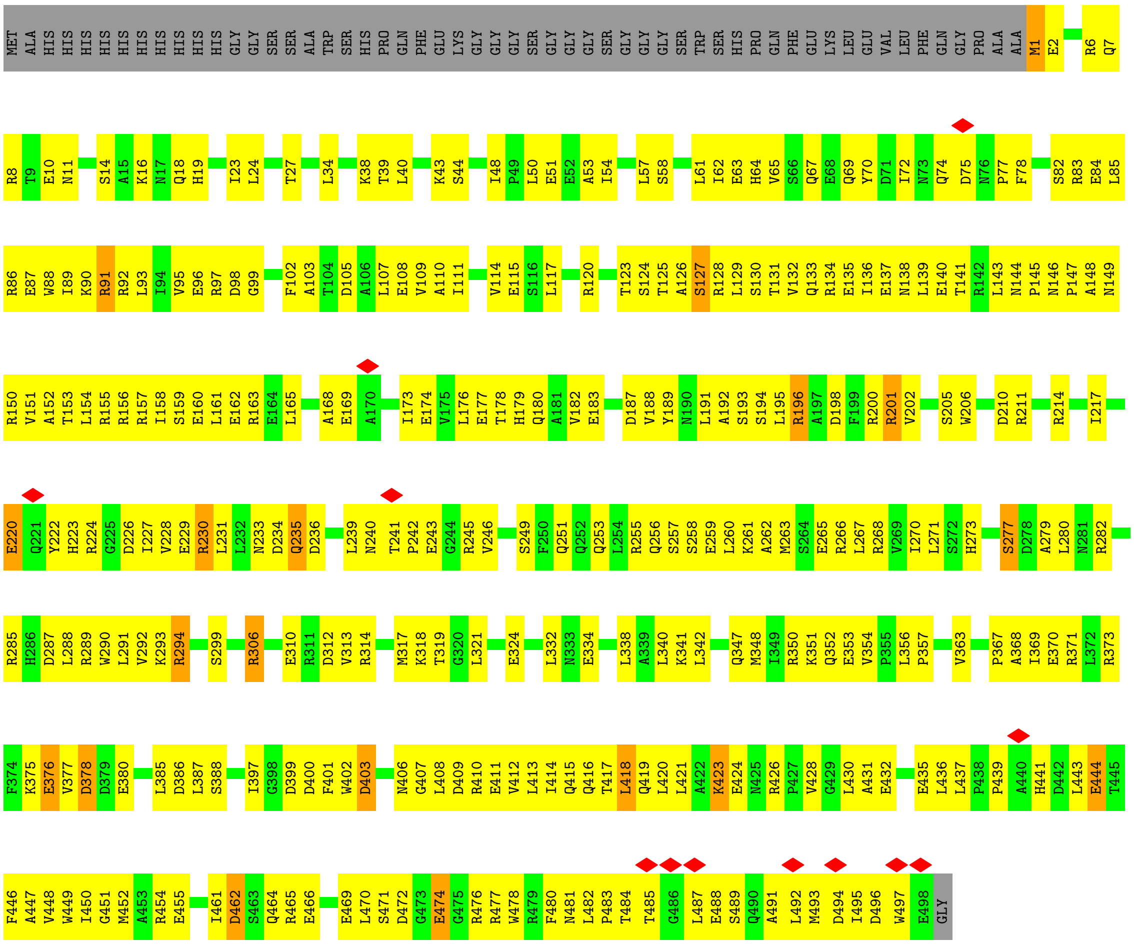
Chain I:





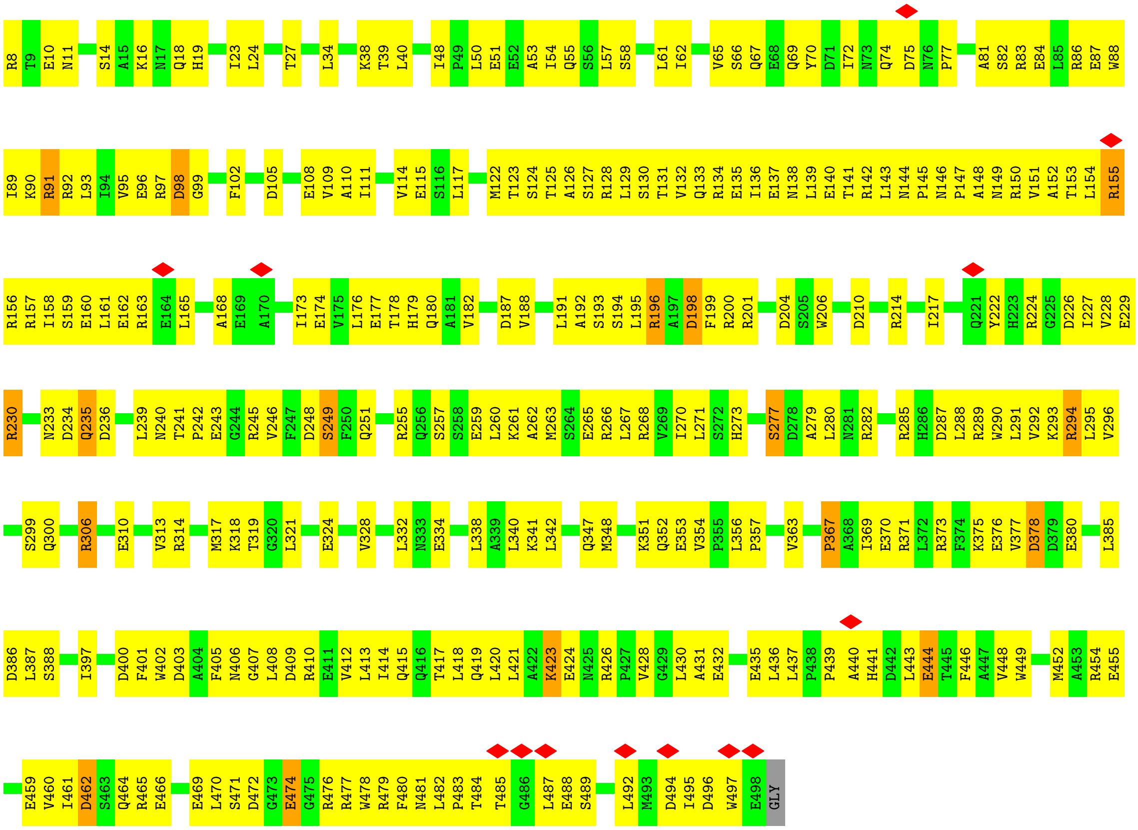
- Molecule 3: JetA

Chain E:



- Molecule 3: JetA

Chain J:


R8 T9 E10 N11 S14 A15 K16 N17 Q18 H19 I23 L24 T27 L34 K38 T39 L40 I48 P49 L50 E51 E52 A53 I54 Q55 S56 L57 S58 L61 I62 V65 S66 Q67 E68 Q69 Y70 D71 I72 N73 Q74 D75 N76 P77 A81 S82 R83 E84 L85 R86 E87 W88
I89 K90 R91 R92 L93 I94 V95 E96 R97 D98 G99 F102 D105 E108 V109 A110 I111 V114 E115 S116 L117 M122 T123 S124 T125 A126 S127 R128 L129 S130 T131 V132 Q133 R134 E135 I136 E137 N138 L139 E140 T141 R142 L143 N144 P145 N146 P147 A148 N149 R150 V151 A152 T153 L154 R155
R156 R157 I158 S159 E160 L161 E162 R163 E164 L165 A168 E169 A170 I173 E174 V175 L176 E177 T178 H179 Q180 A181 V182 D187 V188 L191 A192 S193 S194 L195 R196 A197 D198 F199 R200 R201 D204 S205 W206 D210 R214 I217 Q221 Y222 H223 R224 G225 D226 I227 V228 E229
R230 N233 D234 Q235 D236 L239 N240 T241 P242 E243 G244 R245 V246 F247 D248 S249 F250 Q251 R255 Q256 S257 S258 E259 L260 K261 A262 M263 S264 E265 R266 L267 R268 V269 I270 L271 S272 H273 S277 D278 A279 L280 N281 R282 R285 H286 D287 L288 R289 W290 L291 V292 K293 R294 L295 V296
S299 Q300 R306 E310 V313 R314 M317 K318 T319 G320 L321 E324 V328 L332 N333 E334 L338 A339 L340 K341 L342 Q347 M348 K351 Q352 E353 V354 P355 L356 P357 V363 P367 A368 I369 E370 R371 L372 R373 F374 K375 E376 V377 D378 D379 E380 L385
D386 L387 S388 I397 D400 F401 W402 D403 A404 F405 N406 G407 L408 D409 R410 E411 V412 L413 I414 Q415 Q416 T417 L418 Q419 L420 L421 A422 K423 E424 N425 R426 P427 V428 G429 L430 A431 E432 E435 L436 L437 P438 P439 A440 H441 D442 L443 E444 T445 F446 A447 V448 W449 M452 A453 R454 E455
E459 V460 I461 D462 S463 Q464 R465 E466 E469 L470 S471 D472 G473 E474 G475 R476 R477 W478 R479 F480 N481 L482 P483 T484 T485 G486 L487 E488 S489 L492 M493 D494 I495 D496 W497 E498 GLY

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 $(e^-/\text{Å}^2)$	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	0.28	0/4817	0.51	0/6502
1	B	0.25	0/4817	0.52	0/6502
1	F	0.27	0/4817	0.51	0/6502
1	G	0.24	0/4817	0.49	0/6502
2	C	0.27	0/1592	0.49	0/2164
2	D	0.27	0/1592	0.53	1/2164 (0.0%)
2	H	0.27	0/1592	0.49	0/2164
2	I	0.25	0/1592	0.50	0/2164
3	E	0.26	0/4110	0.53	0/5560
3	J	0.26	0/4110	0.52	1/5560 (0.0%)
All	All	0.26	0/33856	0.51	2/45784 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	198	PRO	CA-N-CD	-6.97	101.73	111.50
3	J	98	ASP	CB-CG-OD1	6.24	123.91	118.30

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	349	0
1	B	4735	0	4689	576	0
1	F	4735	0	4689	349	0
1	G	4735	0	4689	549	0
2	C	1566	0	1605	133	0
2	D	1566	0	1605	123	0
2	H	1566	0	1605	130	0
2	I	1566	0	1605	129	0
3	E	4044	0	4007	482	0
3	J	4044	0	4007	484	0
4	A	27	12	12	1	0
4	B	27	12	12	3	0
4	F	27	12	12	3	0
4	G	27	12	12	2	0
All	All	33400	48	33238	2931	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 44.

All (2931) 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: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
1:F:881:MET:HE1	1:F:894:LEU:HD13	1.42	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
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
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:J:314:ARG:HA	3:J:317:MET:HE2	1.50	0.93
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:J:40:LEU:HD22	3:J:48:ILE:HG21	1.50	0.92
3:E:314:ARG:HA	3:E:317:MET:HE2	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
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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:834:GLU:CD	3:J:241:THR:HB	2.06	0.76
1:B:1085:LEU:HD12	3:E:477:ARG:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
3:E:241:THR:HB	1:F:834:GLU:CD	2.06	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
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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:909:LYS:HA	1:G:912:ARG:HH12	1.57	0.70
1:B:168:LEU:HD13	1:B:171:MET:HE1	1.72	0.70
1:B:866:GLU:O	1:B:870:ILE:HG13	1.92	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
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

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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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
3:E:263:MET:HE2	3:J:133:GLN:HA	1.74	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
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
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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:J:295:LEU:O	3:J:299:SER:OG	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1038:ALA:HA	1:G:1041:GLU:OE1	1.96	0.64
1:B:1020:LEU:CD1	1:B:1023:ALA:HA	2.28	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:52:LEU:HD21	1:A:1077:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:905:ARG:O	1:A:909:LYS:HG3	1.97	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: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
3:E:133:GLN:HA	3:J:263:MET:HE2	1.80	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:66:TYR:O	1:A:76:SER:OG	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:42:THR:HG23	2:I:42:THR:O	1.97	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1056:ARG:HA	1:F:1059:ARG:HB2	1.81	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
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
3:E:266:ARG:HB3	3:J:140:GLU:CD	2.20	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:143:TRP:C	1:G:144:LEU:HD23	2.20	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:801:MET:HE2	1:A:822:ILE:HD11	1.81	0.61
1:A:976:GLU:OE2	1:B:90:PRO:HD2	2.00	0.61

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:975:ILE:HG22	1:B:976:GLU:CD	2.22	0.60
3:E:375:LYS:HD3	3:E:376:GLU:N	2.16	0.60
1:G:1085:LEU:CD1	3:J:477:ARG:HH21	2.13	0.60
1:B:881:MET:HE3	1:B:892:LEU:O	2.00	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:893:ARG:HG2	1:F:894:LEU:N	2.17	0.60
1:G:975:ILE:HG22	1:G:976:GLU:CD	2.22	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:G:30:HIS:HB3	1:G:1077:MET:HE2	1.84	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
3:E:243:GLU:OE1	3:J:122:MET:HE1	2.02	0.59

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:267:LEU:HD22	3:J:136:ILE:CD1	2.33	0.59
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:42:ILE:HD12	1:B:1055:MET:CE	2.32	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:J:263:MET:O	3:J:267:LEU:HD23	2.03	0.58
1:A:61:CYS:O	1:A:184:LYS:NZ	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:79:ASP:OD2	1:G:79:ASP:N	2.35	0.58
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:176:ILE:HD12	2:C:187:ASP:OD2	2.04	0.58
1:A:851:SER:O	1:A:852:SER:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:242:PHE:HZ	1:B:932:GLN:HG3	1.69	0.57
3:E:133:GLN:HA	3:J:263:MET:CE	2.34	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:B:42:ILE:HD12	1:B:1055:MET:HE1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:42:ILE:HD12	1:G:1055:MET:CE	2.35	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
1:G:42:ILE:HD12	1:G:1055:MET:HE1	1.87	0.57
1:G:881:MET:HE1	1:G:893:ARG:HA	1.86	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:LEU:O	1:G:187:TYR:OH	2.20	0.56
1:G:812:LEU:HD23	1:G:824:VAL:CG1	2.34	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:801:MET:HE2	1:F:822:ILE:HD11	1.89	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:32:ALA:HB2	1:A:1077:MET:HE2	1.88	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:B:199:GLU:OE2	1:B:199:GLU:N	2.39	0.55
3:E:133:GLN:OE1	3:J:263:MET:HE2	2.06	0.55
3:E:257:SER:HA	3:E:261:LYS:HZ3	1.71	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:252:LEU:HA	1:G:840:LYS:HZ3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:92:ASP:HB2	1:G:980:GLY:O	2.05	0.55
1:F:881:MET:HE1	1:F:894:LEU:CD1	2.27	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:799:LYS:HB2	1:B:799:LYS:HZ3	1.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:200:ASN:N	1:F:200:ASN:OD1	2.38	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: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: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: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
3:E:472:ASP:CG	3:E:478:TRP:HE1	2.10	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:A:897:LYS:HG2	1:A:898:LYS:N	2.19	0.54
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:12:SER:C	1:F:116:ARG:HD3	2.27	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: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
3:J:84:GLU:HA	3:J:84:GLU:OE2	2.06	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
3:E:243:GLU:HG3	3:J:122:MET:HE3	1.87	0.54
1:F:95:GLU:HG2	1:F:98:SER:H	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:153:THR:HA	3:E:156:ARG:CZ	2.37	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
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:266:ARG:HH12	3:J:137:GLU:CD	2.09	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: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
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
1:B:801:MET:HE1	1:B:817:ALA:HA	1.90	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
1:A:968:ASP:HB2	1:A:971:SER:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:801:MET:HE1	1:F:822:ILE:HG12	1.90	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:A:12:SER:C	1:A:116:ARG:HD3	2.28	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
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:397:ILE:HD13	3:J:401:PHE:CD2	2.43	0.53
3:J:414:ILE:HG12	3:J:452:MET:CE	2.39	0.53
1:B:21:PHE:CE1	1:B:29:LEU:HB2	2.44	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:F:57:MET:HA	1:F:57:MET:HE2	1.89	0.53
1:G:262:LEU:CB	1:G:829:LEU:HD23	2.34	0.53
1:G:938:LEU:CD2	1:G:954:LEU:HD11	2.39	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:227:ASP:OD1	1:B:227:ASP:N	2.42	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
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:E:243:GLU:CD	3:J:122:MET:HE1	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:832:LEU:HD23	1:A:836:ALA:CB	2.38	0.52
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:81:ILE:CD1	1:F:139:MET:HE2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:182:LEU:O	2:I:186:LEU:HG	2.10	0.52
3:J:408:LEU:HD23	3:J:408:LEU:C	2.30	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: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:A:81:ILE:HD13	1:A:139:MET:HE2	1.92	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
1:A:998:THR:HG21	1:A:1039:LEU:HA	1.91	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:G:30:HIS:HB3	1:G:1077:MET:CE	2.40	0.51
1:G:263:GLN:HB2	1:G:264:PRO:HD3	1.91	0.51
1:G:799:LYS:HB2	1:G:799:LYS:HZ3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:92:ASP:C	1:B:981:SER:HB2	2.30	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:201:ARG:HG2	3:E:243:GLU:CD	2.30	0.51
1:G:57:MET:HE2	1:G:206:ASN:HA	1.93	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
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:242:PRO:O	3:E:243:GLU:C	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:ILE:HG12	3:E:452:MET:CE	2.41	0.51
1:F:62:ALA:HB2	1:F:188:LEU:CD1	2.41	0.51
1:F:81:ILE:HD13	1:F:139:MET:HE2	1.91	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:244:GLY:C	1:G:248:ILE:HD12	2.31	0.51
1:G:894:LEU:HB3	1:G:964:VAL:HG22	1.92	0.51
1:G:1058:LEU:O	1:G:1062:THR:OG1	2.17	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: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
2:I:55:LEU:CD1	2:I:61:LEU:HB2	2.41	0.51
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:169:GLU:OE2	3:J:151:VAL:HG11	2.10	0.50
3:E:408:LEU:HD23	3:E:408:LEU:C	2.32	0.50
3:E:414:ILE:HG12	3:E:452:MET:HE1	1.93	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
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:F:92:ASP:C	1:G:981:SER:HB2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:877:LEU:C	1:G:877:LEU:HD13	2.32	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:A:132:THR:O	1:A:132:THR:HG22	2.11	0.50
1:B:79:ASP:OD2	1:B:79:ASP:N	2.45	0.50
1:B:876:GLU:HB3	1:B:1003:TYR:HH	1.77	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:F:808:ASP:CG	1:F:812:LEU:HB2	2.31	0.50
1:G:248:ILE:HD13	1:G:847:TYR:CD2	2.46	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
2:I:137:ARG:HD3	2:I:210:ILE:CG2	2.41	0.50
3:J:240:ASN:CG	3:J:242:PRO:HD2	2.32	0.50
1:B:181:TYR:HD2	1:B:187:TYR:CB	2.24	0.50
1:B:799:LYS:HB2	1:B:799:LYS:NZ	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
1:G:815:ALA:HB1	1:G:821:ASP:CG	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:60:LEU:HD12	2:H:60:LEU:C	2.32	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: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
1:G:881:MET:CE	1:G:893:ARG:HA	2.41	0.49
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:30:HIS:HB3	1:B:1077:MET:CE	2.43	0.49
1:B:792:ARG:NH1	1:B:792:ARG:CB	2.76	0.49
1:B:805:LYS:HA	1:B:808:ASP:CG	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:MET:HE2	1:B:206:ASN:HA	1.94	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: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: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
3:E:163:ARG:CZ	3:E:163:ARG:HB2	2.43	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
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:815:ALA:HB1	1:B:821:ASP:CG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:60:LEU:HD12	2:D:60:LEU:C	2.33	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
2:H:45:LEU:HD13	2:H:48:ILE:CD1	2.30	0.49
3:J:242:PRO:O	3:J:243:GLU:C	2.49	0.49
1:A:228:ASP:HA	1:A:957:ARG:NH2	2.28	0.48
1:B:851:SER:O	1:B:852:SER:HB2	2.13	0.48
2:D:55:LEU:O	2:D:59:GLY:N	2.41	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:1029:HIS:C	1:G:1029:HIS:ND1	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:60:LEU:C	2:I:60:LEU:HD12	2.33	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:233:ASN:CG	3:J:235:GLN:H	2.15	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:A:801:MET:HE1	1:A:822:ILE:HG12	1.94	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
1:G:876:GLU:HA	1:G:879:GLU:CD	2.34	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:247:GLU:HA	1:B:250:GLN:CD	2.34	0.48
1:B:252:LEU:HA	1:B:840:LYS:HZ3	1.78	0.48
1:B:953:LEU:C	1:B:954:LEU:HD12	2.33	0.48
3:E:151:VAL:HG13	3:J:165:LEU:HD21	1.96	0.48
3:E:378:ASP:OD1	3:E:378:ASP:C	2.52	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
1:G:126:LEU:C	1:G:127:LEU:HD22	2.34	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
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
2:I:215:ASP:CG	2:I:215:ASP:O	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:F:168:LEU:HD23	1:F:171:MET:HE2	1.96	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:378:ASP:C	3:J:378:ASP:OD1	2.52	0.48
3:J:482:LEU:N	3:J:482:LEU:HD12	2.29	0.48
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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:914:LEU:HD23	1:G:914:LEU:C	2.35	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
1:B:1080:LEU:HD23	1:B:1080:LEU:C	2.35	0.47
3:E:200:ARG:HD2	3:E:200:ARG:N	2.29	0.47
1:F:32:ALA:HB2	1:F:1077:MET:CE	2.43	0.47
1:F:875:ASN:C	1:F:875:ASN:OD1	2.52	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
1:G:953:LEU:C	1:G:954:LEU:HD12	2.34	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: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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLY:O	1:B:49:LYS:NZ	2.39	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: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: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:C:121:ARG:O	2:C:122:ARG:HB2	2.15	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:1059:ARG:HB2	3:J:443:LEU:HD22	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
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:52:LEU:HD11	1:A:1077:MET:HE3	1.96	0.46
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:O	1:B:914:LEU:HD23	2.15	0.46
2:C:106:LEU:O	2:C:106:LEU:HD12	2.14	0.46
3:E:154:LEU:CA	3:J:161:LEU:HD21	2.45	0.46
3:E:233:ASN:CG	3:E:235:GLN:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:914:LEU:HD23	1:B:914:LEU:C	2.35	0.46
1:B:995:TYR:HH	1:B:1042:PHE:HE2	1.62	0.46
2:C:85:GLU:HG2	2:D:43:ARG:HH21	1.80	0.46
2:D:105:ARG:O	2:D:105:ARG:HG2	2.14	0.46
3:E:257:SER:HA	3:E:261:LYS:HZ1	1.80	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
1:B:142:LEU:HD13	1:B:142:LEU:C	2.36	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
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: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
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
3:E:135:GLU:OE1	3:J:135:GLU:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:783:ILE:O	1:F:787:LYS:HG2	2.15	0.46
1:G:220:ILE:HD11	1:G:993:ALA:HB1	1.98	0.46
2:H:156:ILE:HG13	2:H:156:ILE:O	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:185:LYS:HD3	1:A:185:LYS:HA	1.65	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: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
3:E:431:ALA:H	3:E:466:GLU:CD	2.14	0.46
1:F:1057:LEU:HD12	1:F:1057:LEU:C	2.34	0.46
1:G:1086:GLU:O	1:G:1087:ARG:C	2.54	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
1:B:787:LYS:O	1:B:787:LYS:HD3	2.16	0.46
1:B:796:GLU:CD	1:B:800:ARG:HD3	2.36	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: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
1:G:967:MET:HE2	1:G:972:GLY:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:I:44:THR:H	2:I:44:THR:HG1	1.56	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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:782:GLU:N	1:A:782:GLU:OE1	2.48	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
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:A:59:LEU:O	1:A:187:TYR:OH	2.29	0.45
1:B:845:LEU:HA	1:B:848:LEU:CD2	2.46	0.45
1:B:877:LEU:C	1:B:877:LEU:HD13	2.36	0.45
1:B:1084:GLU:HB2	3:E:478:TRP:HZ3	1.79	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
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:65:SER:C	2:D:66:LYS:HD2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1080:LEU:HD23	1:G:1080:LEU:C	2.37	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:81:ILE:HD13	1:A:139:MET:CE	2.47	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
2:D:187:ASP:C	2:D:187:ASP:OD1	2.55	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: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: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
3:E:155:ARG:HG2	3:J:165:LEU:HD23	1.99	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:914:LEU:HD23	1:G:914:LEU:O	2.17	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
1:B:1086:GLU:O	1:B:1087:ARG:C	2.55	0.45
3:E:157:ARG:HB3	3:J:161:LEU:CD1	2.36	0.45
1:F:196:GLU:OE1	2:H:177:LYS:NZ	2.36	0.45
1:F:1054:GLU:HG2	1:F:1057:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:881:MET:HE1	1:B:892:LEU:HG	1.99	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
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:192:ARG:HD2	1:B:198:GLY:C	2.38	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:234:ARG:HA	1:B:237:GLU:CD	2.36	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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: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
3:E:243:GLU:CG	3:J:122:MET:HE3	2.47	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: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
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: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:217:ILE:HD11	1:G:962:PHE:C	2.37	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
2:I:187:ASP:C	2:I:187:ASP:OD1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:E:133:GLN:OE1	3:J:263:MET:CE	2.66	0.44
1:F:90:PRO:HD2	4:F:1101:ADP:N3	2.33	0.44
1:G:30:HIS:CB	1:G:1077:MET:HE2	2.47	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
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
2:D:215:ASP:CG	2:D:215:ASP:O	2.56	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: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:81:ILE:CD1	1:A:139:MET:HE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:ILE:HD12	1:A:1066:ILE:N	2.33	0.44
1:B:168:LEU:HD13	1:B:171:MET:HE2	1.98	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:153:LEU:HD23	1:G:153:LEU:C	2.38	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
2:I:65:SER:C	2:I:66:LYS:HD2	2.38	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
1:A:100:ILE:O	1:A:100:ILE:HG22	2.18	0.43
1:A:824:VAL:CG2	1:A:825:TYR:N	2.81	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
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: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:1086:GLU:HG3	1:A:1087:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:55:GLN:OE1	3:J:55:GLN:HA	2.18	0.43
3:J:263:MET:C	3:J:267:LEU:HD23	2.38	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:52:LEU:HD11	1:F:1077:MET:CE	2.47	0.43
1:F:65:ARG:N	1:F:206:ASN:HD21	2.16	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
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: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:57:MET:HA	1:F:57:MET:CE	2.48	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:472:ASP:CG	3:J:478:TRP:HE1	2.22	0.43
1:A:282:TRP:CE3	1:A:783:ILE:HD12	2.54	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
3:E:293:LYS:HZ3	3:E:293:LYS:HB2	1.84	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
3:J:414:ILE:HG12	3:J:452:MET:HE2	2.01	0.43
1:A:266:ALA:O	1:A:270:GLU:HG3	2.18	0.43
1:B:1031:VAL:O	1:B:1035:ILE:CD1	2.59	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
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: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:421:LEU:C	3:E:489:SER:HB2	2.39	0.43
1:F:100:ILE:O	1:F:100:ILE:HG22	2.18	0.43
1:F:797:LEU:HD12	1:F:801:MET:HE2	2.00	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
1:G:34:ILE:HG23	1:G:39:THR:HG21	2.00	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:138:ASN:OD1	3:J:138:ASN:C	2.58	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:57:MET:HA	1:A:57:MET:CE	2.49	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: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:287:ASP:OD1	3:E:287:ASP:C	2.58	0.42
1:F:18:ILE:HD11	1:F:56:LEU:HD12	2.01	0.42
1:F:1016:GLY:O	1:F:1045:HIS:N	2.52	0.42
1:G:835:GLU:C	1:G:838:PRO:HD2	2.40	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
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:F:1084:GLU:OE1	2:I:174:SER:OG	2.24	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:148:ALA:HA	3:E:151:VAL:CG2	2.49	0.42
1:F:233:ASP:OD1	1:F:233:ASP:C	2.58	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
1:G:995:TYR:HH	1:G:1042:PHE:HE2	1.65	0.42
2:H:124:ARG:HB2	3:J:353:GLU:CG	2.47	0.42
2:H:199:ASP:C	2:H:199:ASP:OD1	2.57	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:848:LEU:HD12	1:B:848:LEU:C	2.40	0.42
2:C:199:ASP:C	2:C:199:ASP:OD1	2.58	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
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:126:LEU:HD11	1:G:157:LEU:HD13	2.02	0.42
1:G:899:VAL:HG12	1:G:959:ARG:C	2.40	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
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: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
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:842:ASN:O	1:B:845:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:LEU:HD23	2:C:74:LEU:HA	1.82	0.42
3:E:259:GLU:H	3:E:259:GLU:CD	2.22	0.42
1:F:895:ASP:OD1	1:F:896:THR:N	2.52	0.42
2:I:209:ILE:CD1	3:J:369:ILE:HG21	2.33	0.42
3:J:287:ASP:OD1	3:J:287:ASP:C	2.58	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
1:B:887:GLN:O	1:B:888:PRO:C	2.58	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: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: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
3:J:414:ILE:HG12	3:J:452:MET:HE1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:30:HIS:HB3	1:B:1077:MET:HE2	2.01	0.41
1:B:790:LEU:O	1:B:790:LEU:HD23	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
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
1:A:261:SER:O	1:A:264:PRO:HG2	2.20	0.41
1:A:921:ASP:C	1:A:921:ASP:OD1	2.58	0.41
2:C:117:HIS:HE1	2:C:119:LEU:HB2	1.85	0.41
3:E:85:LEU:HD23	3:E:85:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:981:SER:O	1:F:982:GLN:C	2.59	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: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:A:801:MET:CE	1:A:822:ILE:HD11	2.49	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: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:783:ILE:HG23	1:G:784:GLU:OE1	2.20	0.41
1:G:805:LYS:HA	1:G:808:ASP:CG	2.40	0.41
1:G:881:MET:HE1	1:G:893:ARG:CA	2.51	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:I:179:ARG:HG3	2:I:179:ARG:HH11	1.85	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:980:GLY:O	1:A:981:SER:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:GLU:HA	1:B:879:GLU:CD	2.40	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
2:C:45:LEU:HD13	2:C:48:ILE:CD1	2.33	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
1:F:143:TRP:CH2	1:F:184:LYS:HE3	2.56	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: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:32:ALA:HB2	1:F:1077:MET:HE2	2.03	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:233:ASP:OD1	1:A:233:ASP:C	2.58	0.41
1:A:832:LEU:CD2	1:A:836:ALA:HB3	2.49	0.41
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:792:ARG:HH11	1:B:792:ARG:HB3	1.86	0.41
1:B:899:VAL:HG12	1:B:959:ARG:C	2.41	0.41
1:B:914:LEU:CD1	1:B:931:LEU:HD22	2.51	0.41
1:B:989:LYS:HD2	1:B:989:LYS:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:PRO:HD2	1:B:1010:SER:HB3	2.03	0.41
1:B:1054:GLU:CD	1:B:1057:LEU:HD21	2.41	0.41
2:C:46:GLN:C	2:C:46:GLN:OE1	2.59	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:243:GLU:CD	3:J:122:MET:CE	2.89	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:H:46:GLN:C	2:H:46:GLN:OE1	2.59	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:121:ARG:HH22	2:D:123:GLN:CD	2.24	0.41
2:D:223:LEU:HD12	2:D:223:LEU:HA	1.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:97:ARG:O	3:J:98:ASP:HB3	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:790:LEU:HD23	1:B:790:LEU:C	2.41	0.40
1:B:842:ASN:HA	1:B:845:LEU:HG	2.03	0.40
3:E:189:TYR:CD1	3:E:189:TYR:C	2.94	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LEU:O	1:F:187:TYR:OH	2.33	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
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: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:829:LEU:C	1:B:829:LEU:HD13	2.42	0.40
1:B:967:MET:HE2	1:B:972:GLY:O	2.20	0.40
1:B:994:SER:O	1:B:998:THR:HG23	2.21	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:275:GLN:HB3	1:F:790:LEU:HD21	2.02	0.40
1:G:881:MET:HE1	1:G:892:LEU:HG	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
2:I:226:LEU:HD23	2:I:226:LEU:HA	1.79	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/1096 (54%)	557 (94%)	35 (6%)	1 (0%)	47	80
1	B	593/1096 (54%)	557 (94%)	32 (5%)	4 (1%)	22	62
1	F	593/1096 (54%)	557 (94%)	35 (6%)	1 (0%)	47	80
1	G	593/1096 (54%)	565 (95%)	26 (4%)	2 (0%)	41	75
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%)	50	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	SER
1	B	1087	ARG
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%)	484 (97%)	17 (3%)	37	68
1	B	501/929 (54%)	479 (96%)	22 (4%)	28	62
1	F	501/929 (54%)	484 (97%)	17 (3%)	37	68
1	G	501/929 (54%)	472 (94%)	29 (6%)	20	54
2	C	171/218 (78%)	168 (98%)	3 (2%)	59	81
2	D	171/218 (78%)	161 (94%)	10 (6%)	20	54
2	H	171/218 (78%)	166 (97%)	5 (3%)	42	71
2	I	171/218 (78%)	163 (95%)	8 (5%)	26	60
3	E	435/474 (92%)	406 (93%)	29 (7%)	16	49
3	J	435/474 (92%)	410 (94%)	25 (6%)	20	54
All	All	3558/5536 (64%)	3393 (95%)	165 (5%)	31	61

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	67	ASN
1	A	120	GLN
1	A	130	ASP
1	A	138	ASP
1	A	185	LYS
1	A	221	PHE
1	A	277	ARG
1	A	282	TRP
1	A	782	GLU
1	A	785	ARG
1	A	891	TYR
1	A	969	ARG
1	A	970	GLN
1	A	1029	HIS
1	A	1070	ARG

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Mol	Chain	Res	Type
1	A	1092	ARG
1	B	74	HIS
1	B	119	LYS
1	B	199	GLU
1	B	212	LYS
1	B	216	SER
1	B	242	PHE
1	B	256	ARG
1	B	281	ASP
1	B	799	LYS
1	B	819	LEU
1	B	820	ASP
1	B	854	ASP
1	B	865	HIS
1	B	875	ASN
1	B	901	HIS
1	B	918	ARG
1	B	969	ARG
1	B	978	ARG
1	B	1021	ASP
1	B	1026	ARG
1	B	1057	LEU
1	B	1059	ARG
2	C	76	HIS
2	C	159	ASP
2	C	161	LEU
2	D	76	HIS
2	D	101	TYR
2	D	107	ASP
2	D	108	GLU
2	D	137	ARG
2	D	168	TYR
2	D	212	HIS
2	D	213	LEU
2	D	215	ASP
2	D	218	ASN
3	E	1	MET
3	E	75	ASP
3	E	91	ARG
3	E	127	SER
3	E	193	SER
3	E	196	ARG

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Mol	Chain	Res	Type
3	E	201	ARG
3	E	205	SER
3	E	220	GLU
3	E	222	TYR
3	E	230	ARG
3	E	235	GLN
3	E	240	ASN
3	E	277	SER
3	E	294	ARG
3	E	306	ARG
3	E	348	MET
3	E	376	GLU
3	E	378	ASP
3	E	386	ASP
3	E	403	ASP
3	E	411	GLU
3	E	418	LEU
3	E	423	LYS
3	E	444	GLU
3	E	462	ASP
3	E	474	GLU
3	E	494	ASP
3	E	496	ASP
1	F	1	MET
1	F	37	ASP
1	F	120	GLN
1	F	138	ASP
1	F	139	MET
1	F	187	TYR
1	F	221	PHE
1	F	277	ARG
1	F	282	TRP
1	F	782	GLU
1	F	785	ARG
1	F	830	GLN
1	F	969	ARG
1	F	970	GLN
1	F	977	SER
1	F	997	LEU
1	F	1029	HIS
1	G	54	ASP
1	G	74	HIS

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Mol	Chain	Res	Type
1	G	79	ASP
1	G	119	LYS
1	G	199	GLU
1	G	212	LYS
1	G	219	GLU
1	G	281	ASP
1	G	799	LYS
1	G	808	ASP
1	G	819	LEU
1	G	820	ASP
1	G	854	ASP
1	G	865	HIS
1	G	875	ASN
1	G	891	TYR
1	G	918	ARG
1	G	932	GLN
1	G	942	CYS
1	G	969	ARG
1	G	978	ARG
1	G	1002	SER
1	G	1021	ASP
1	G	1026	ARG
1	G	1029	HIS
1	G	1057	LEU
1	G	1059	ARG
1	G	1077	MET
1	G	1079	SER
2	H	45	LEU
2	H	68	ASN
2	H	146	GLU
2	H	147	SER
2	H	175	GLU
2	I	101	TYR
2	I	107	ASP
2	I	108	GLU
2	I	137	ARG
2	I	168	TYR
2	I	176	SER
2	I	215	ASP
2	I	226	LEU
3	J	1	MET
3	J	75	ASP

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Mol	Chain	Res	Type
3	J	91	ARG
3	J	155	ARG
3	J	193	SER
3	J	196	ARG
3	J	198	ASP
3	J	222	TYR
3	J	230	ARG
3	J	235	GLN
3	J	249	SER
3	J	277	SER
3	J	294	ARG
3	J	306	ARG
3	J	348	MET
3	J	367	PRO
3	J	378	ASP
3	J	386	ASP
3	J	403	ASP
3	J	423	LYS
3	J	444	GLU
3	J	462	ASP
3	J	474	GLU
3	J	494	ASP
3	J	496	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	937	GLN
1	B	120	GLN
1	B	151	GLN
1	B	273	GLN
1	B	278	GLN
1	B	858	GLN
1	B	901	HIS
1	B	937	GLN
3	E	18	GLN
3	E	415	GLN
1	F	67	ASN
1	F	206	ASN
1	F	830	GLN
1	F	937	GLN

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Mol	Chain	Res	Type
1	G	120	GLN
1	G	151	GLN
1	G	273	GLN
1	G	278	GLN
1	G	858	GLN
1	G	937	GLN
3	J	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	24,29,29	1.94	8 (33%)	29,45,45	1.46	6 (20%)
4	ADP	A	1101	-	24,29,29	1.92	8 (33%)	29,45,45	1.40	5 (17%)
4	ADP	B	1101	-	24,29,29	1.94	8 (33%)	29,45,45	1.44	5 (17%)
4	ADP	F	1101	-	24,29,29	1.93	8 (33%)	29,45,45	1.39	5 (17%)

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	-	-	7/12/32/32	0/3/3/3
4	ADP	A	1101	-	-	6/12/32/32	0/3/3/3
4	ADP	B	1101	-	-	5/12/32/32	0/3/3/3
4	ADP	F	1101	-	-	7/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ADP	O4'-C1'	4.90	1.47	1.41
4	B	1101	ADP	O4'-C1'	4.86	1.47	1.41
4	G	1101	ADP	O4'-C1'	4.85	1.47	1.41
4	F	1101	ADP	O4'-C1'	4.83	1.47	1.41
4	G	1101	ADP	C6-N6	3.15	1.45	1.34
4	B	1101	ADP	C6-N6	3.15	1.45	1.34
4	F	1101	ADP	C6-N6	3.15	1.45	1.34
4	A	1101	ADP	C6-N6	3.12	1.45	1.34
4	B	1101	ADP	C2'-C1'	-2.81	1.49	1.53
4	G	1101	ADP	C2'-C1'	-2.80	1.49	1.53
4	F	1101	ADP	C2'-C1'	-2.60	1.49	1.53
4	A	1101	ADP	C2'-C1'	-2.53	1.49	1.53
4	A	1101	ADP	C2'-C3'	-2.37	1.46	1.53
4	G	1101	ADP	C2'-C3'	-2.36	1.46	1.53
4	F	1101	ADP	C2'-C3'	-2.35	1.46	1.53
4	B	1101	ADP	C2'-C3'	-2.33	1.47	1.53
4	A	1101	ADP	PB-O2B	-2.27	1.46	1.54
4	F	1101	ADP	PB-O2B	-2.27	1.46	1.54
4	F	1101	ADP	PB-O3B	-2.25	1.46	1.54
4	B	1101	ADP	C5-N7	2.24	1.47	1.39
4	A	1101	ADP	C5-N7	2.24	1.47	1.39
4	G	1101	ADP	C5-N7	2.24	1.47	1.39
4	A	1101	ADP	PB-O3B	-2.24	1.46	1.54
4	F	1101	ADP	C5-N7	2.24	1.47	1.39
4	B	1101	ADP	PB-O3B	-2.21	1.46	1.54
4	G	1101	ADP	PB-O3B	-2.21	1.46	1.54
4	G	1101	ADP	C4-N3	-2.20	1.32	1.35
4	B	1101	ADP	C4-N3	-2.20	1.32	1.35
4	G	1101	ADP	PB-O2B	-2.20	1.46	1.54
4	B	1101	ADP	PB-O2B	-2.19	1.46	1.54
4	F	1101	ADP	C4-N3	-2.16	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ADP	C4-N3	-2.08	1.32	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1101	ADP	C3’-C2’-C1’	3.56	106.34	100.98
4	B	1101	ADP	C3’-C2’-C1’	3.45	106.17	100.98
4	A	1101	ADP	C3’-C2’-C1’	3.31	105.96	100.98
4	F	1101	ADP	PA-O3A-PB	-3.18	121.90	132.83
4	F	1101	ADP	C3’-C2’-C1’	3.17	105.75	100.98
4	A	1101	ADP	PA-O3A-PB	-3.12	122.11	132.83
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	G	1101	ADP	PA-O3A-PB	-2.78	123.28	132.83
4	B	1101	ADP	O2B-PB-O3A	2.78	113.95	104.64
4	B	1101	ADP	PA-O3A-PB	-2.77	123.33	132.83
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	O2A-PA-O1A	-2.27	101.04	112.24
4	B	1101	ADP	O2A-PA-O1A	-2.26	101.07	112.24
4	A	1101	ADP	O2A-PA-O1A	-2.17	101.53	112.24
4	F	1101	ADP	O2A-PA-O1A	-2.16	101.54	112.24
4	G	1101	ADP	C2’-C3’-C4’	2.05	106.63	102.64

There are no chirality outliers.

All (25) 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	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	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	C5’-O5’-PA-O3A
4	A	1101	ADP	PB-O3A-PA-O2A

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

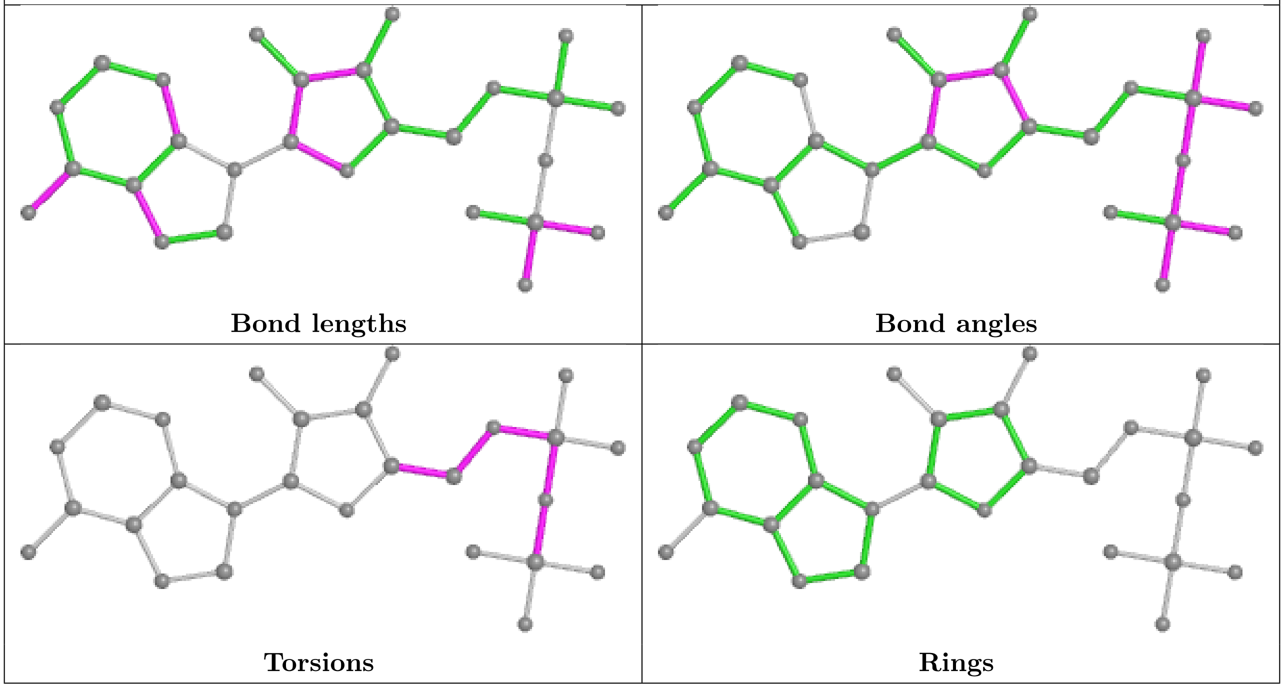
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1101	ADP	2	0
4	A	1101	ADP	1	0
4	B	1101	ADP	3	0
4	F	1101	ADP	3	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 then 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.

Ligand ADP G 1101



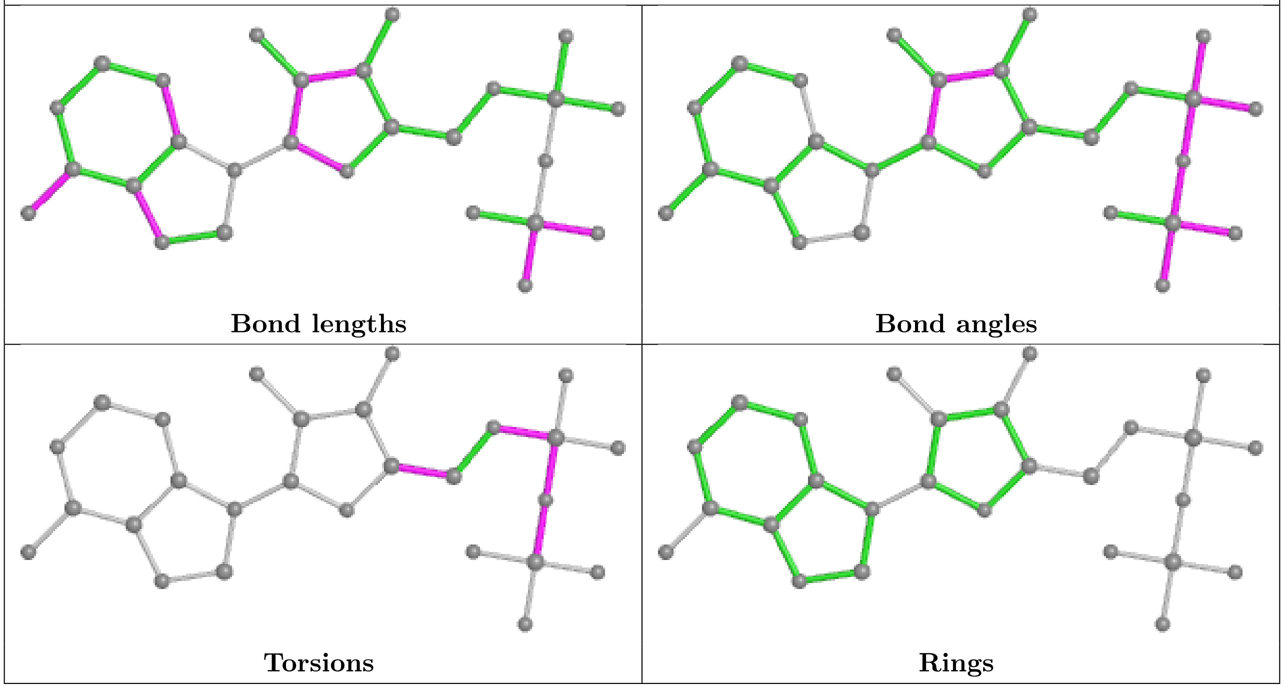
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1101



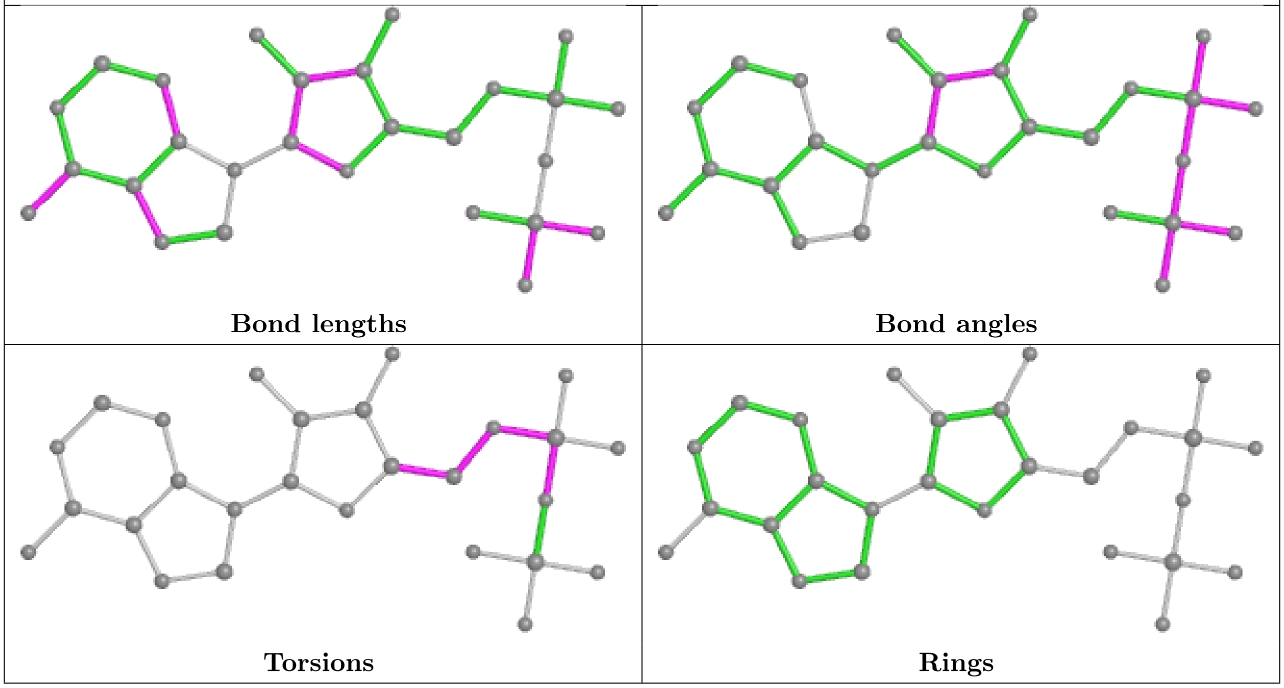
Bond lengths

Bond angles

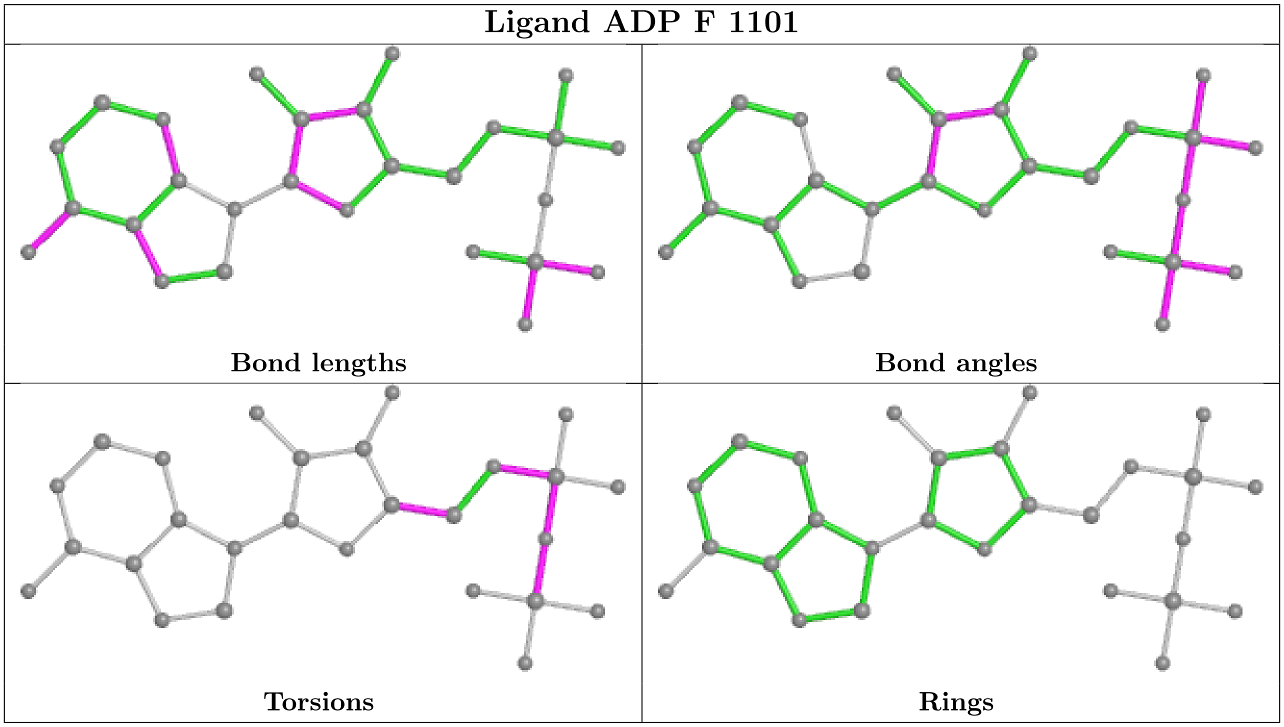
Torsions

Rings

Ligand ADP B 1101



Ligand ADP F 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

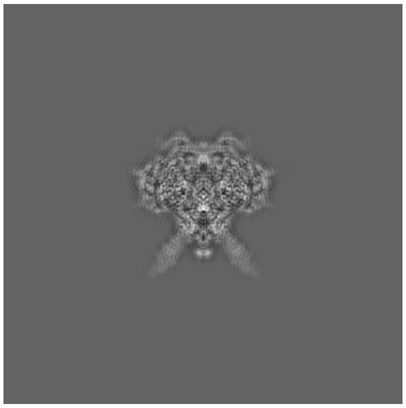
6 Map visualisation

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

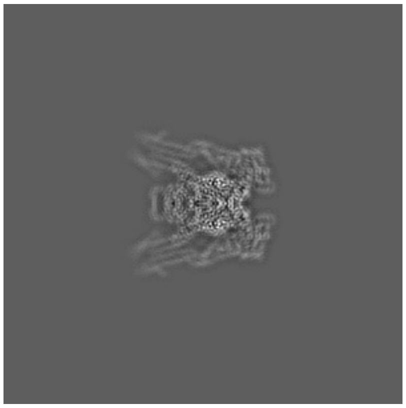
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

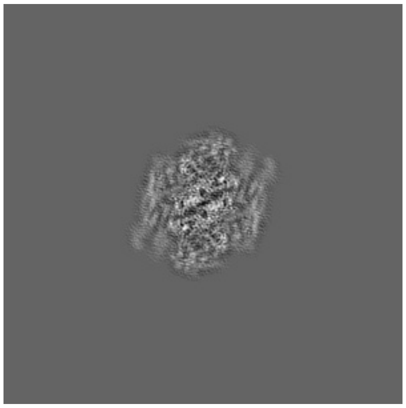
6.1.1 Primary map



X

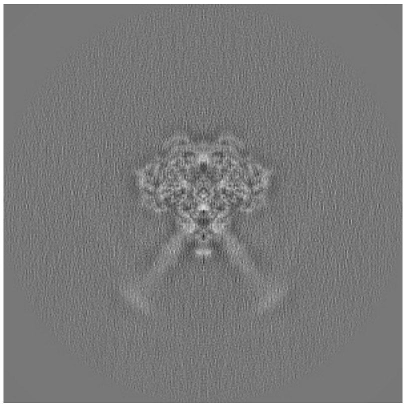


Y

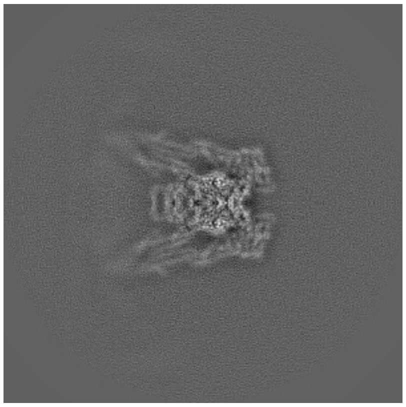


Z

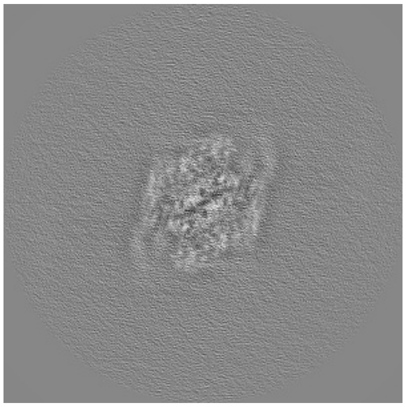
6.1.2 Raw map



X



Y

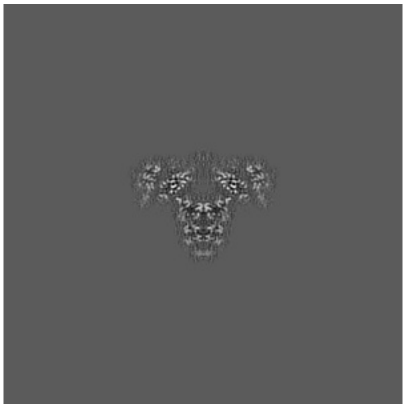


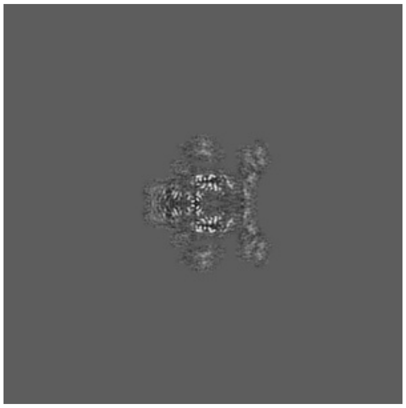
Z

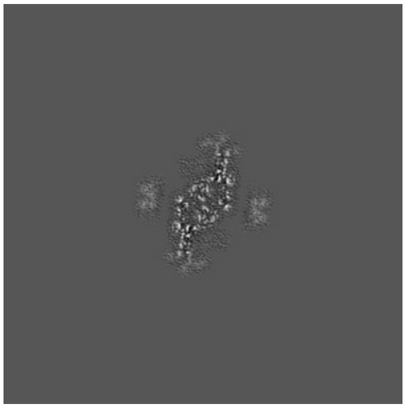
The images above show the map projected in three orthogonal directions.

6.2 Central slices

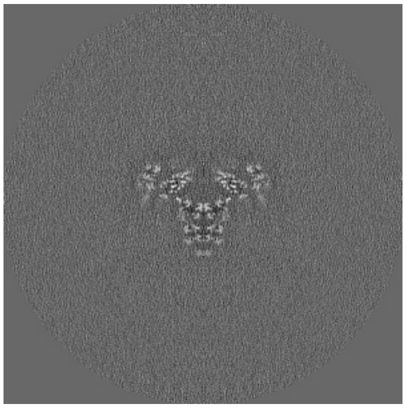
6.2.1 Primary map

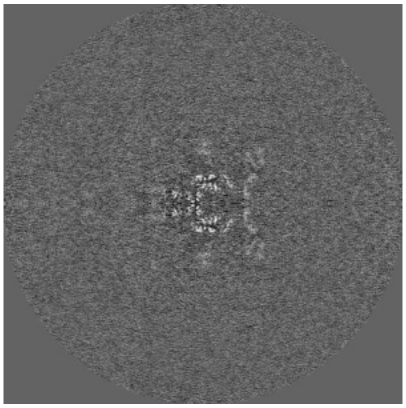

X Index: 200

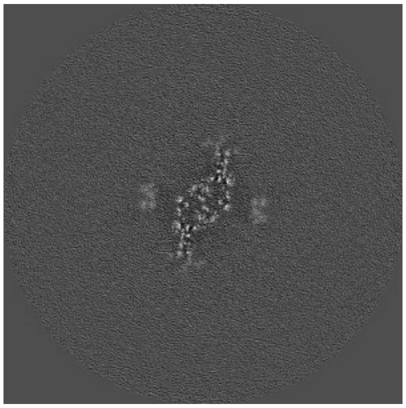

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

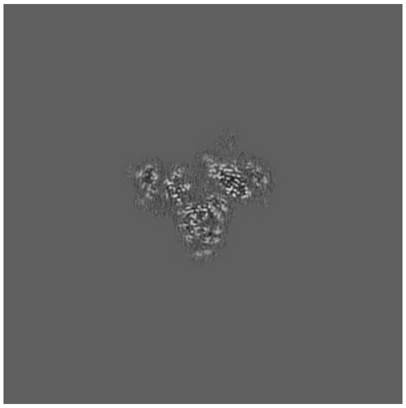

Y Index: 200

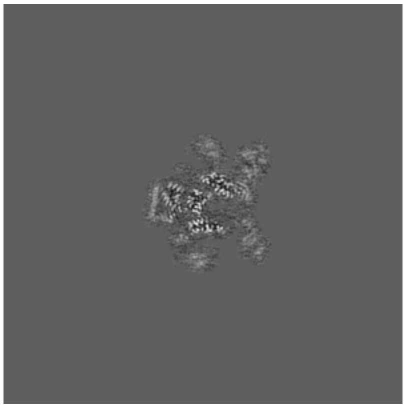

Z Index: 200

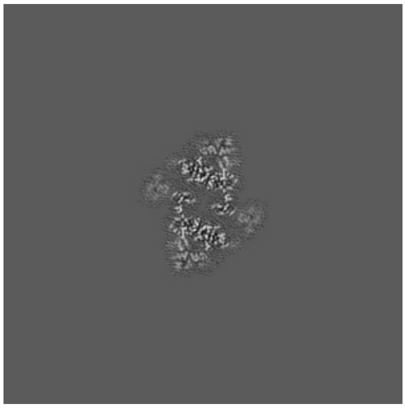
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

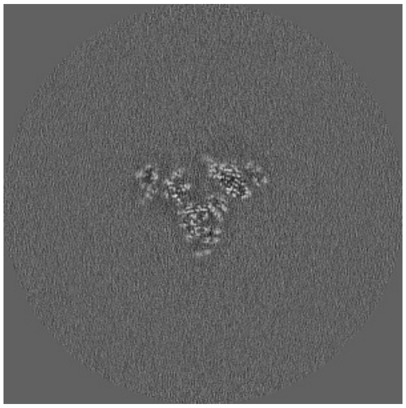
6.3.1 Primary map

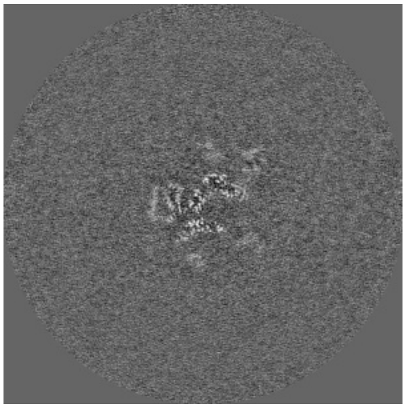

X Index: 195

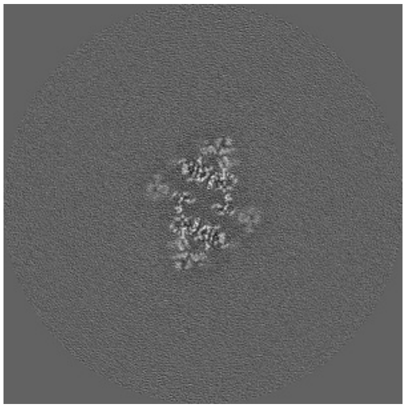

Y Index: 196


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.

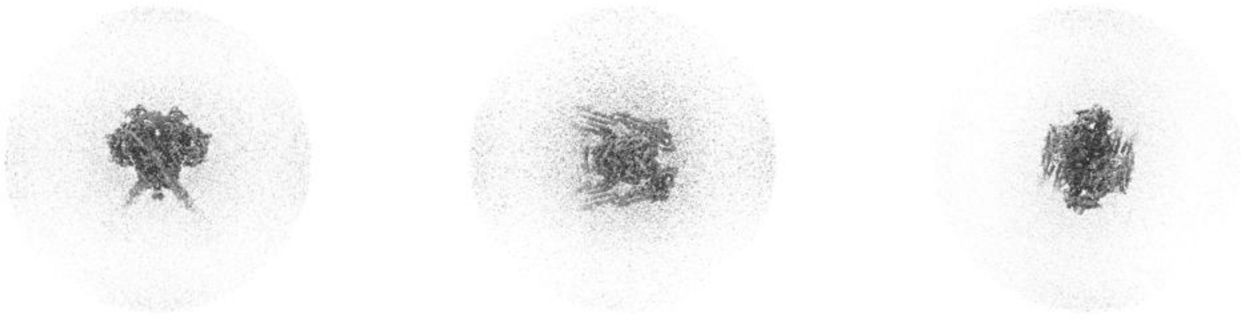
6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00296. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

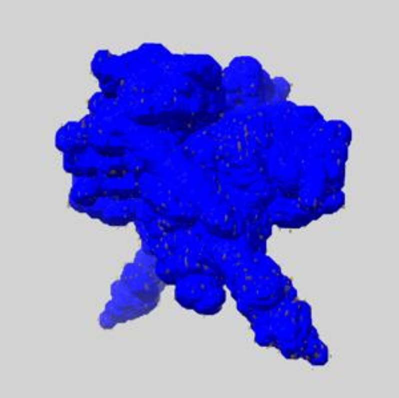
6.5 Mask visualisation ⓘ

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

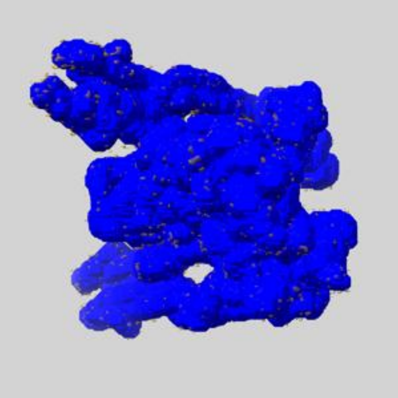
A mask typically either:

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

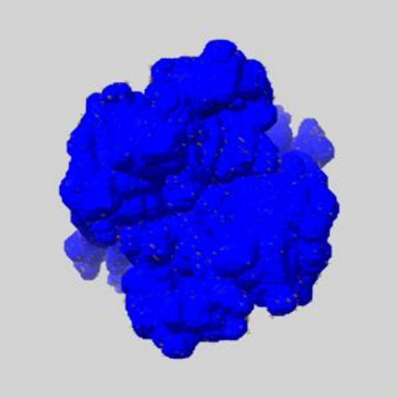
6.5.1 emd_16020_msk_1.map ⓘ



X



Y

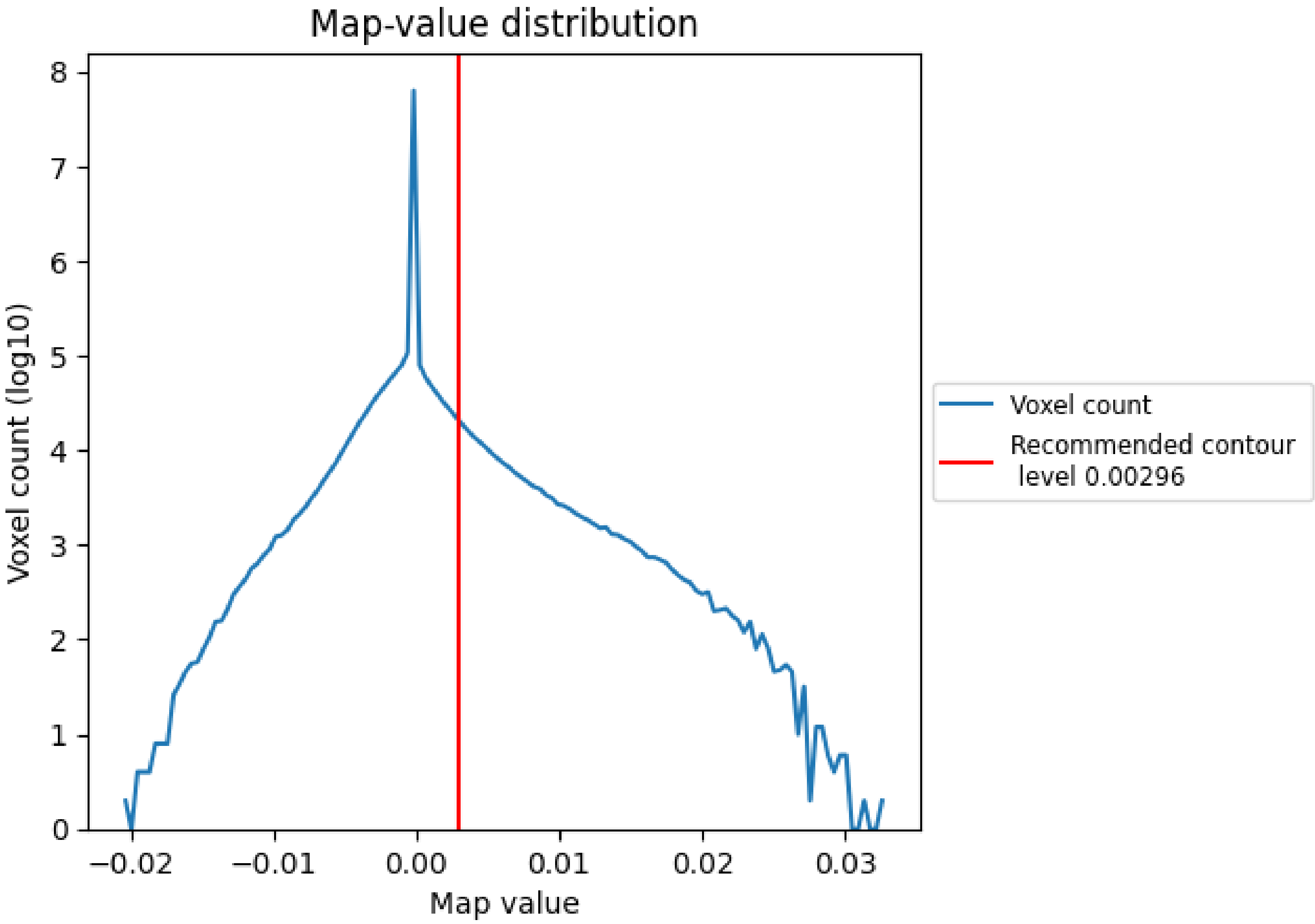


Z

7 Map analysis ⓘ

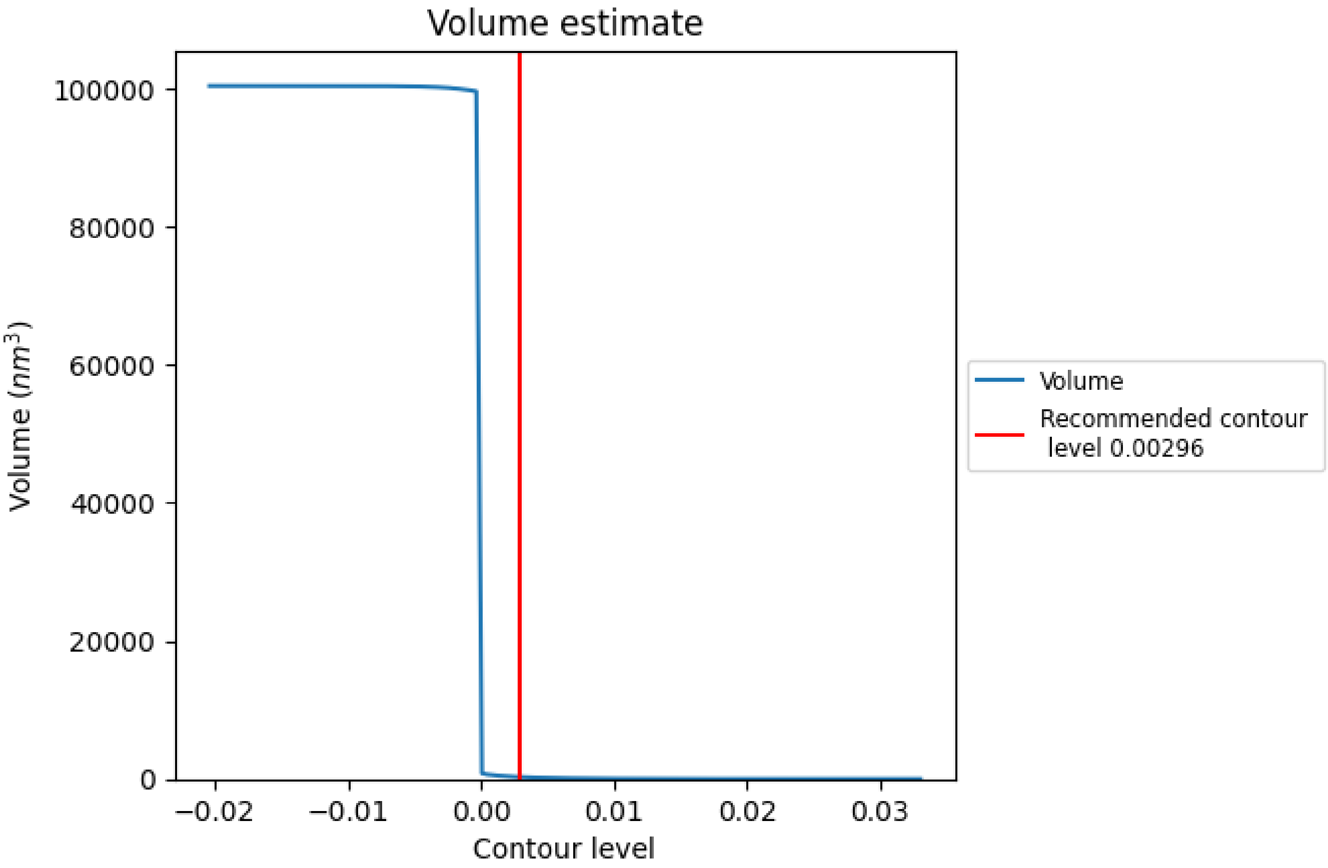
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

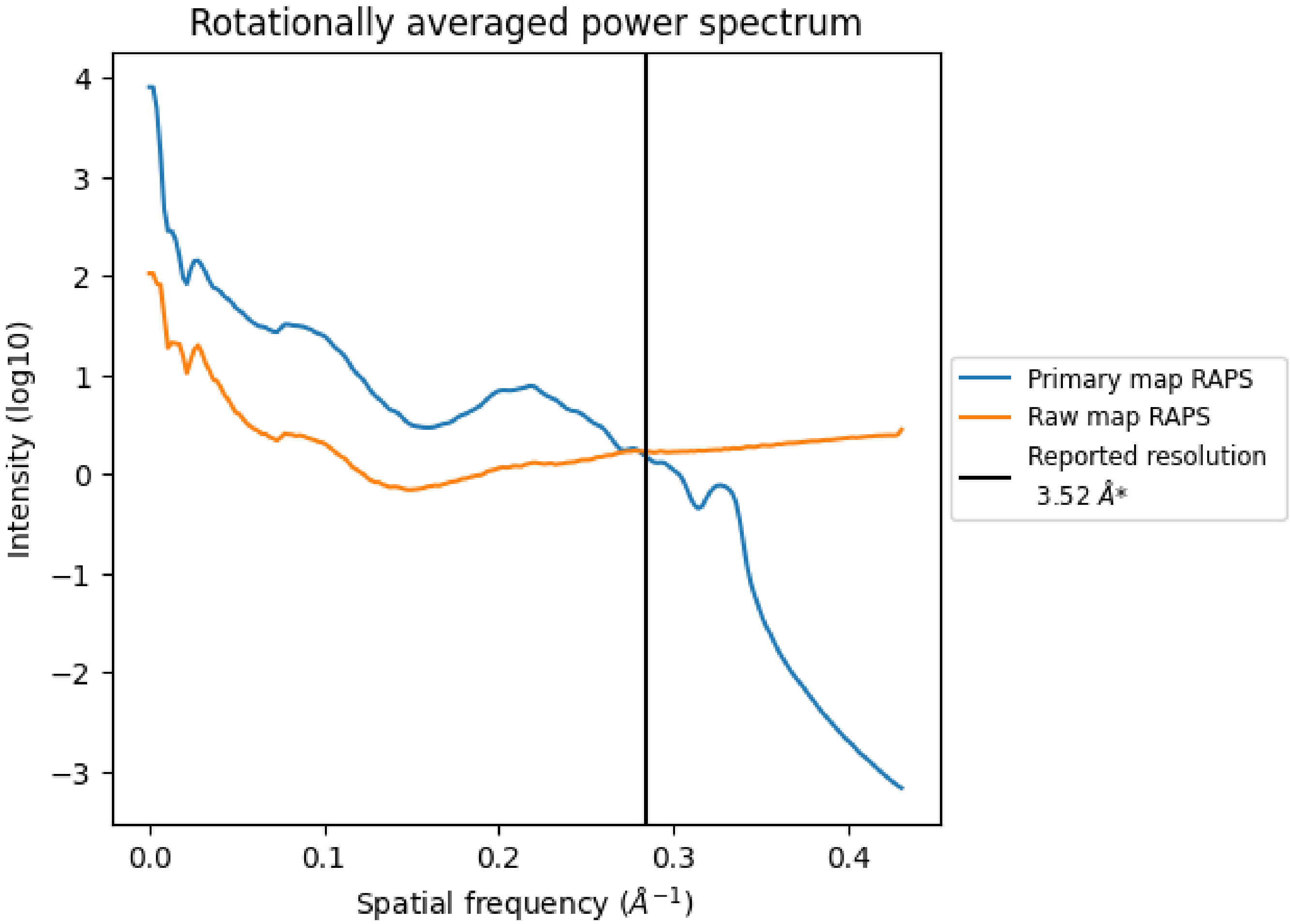
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 278 nm^3; 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 ⓘ

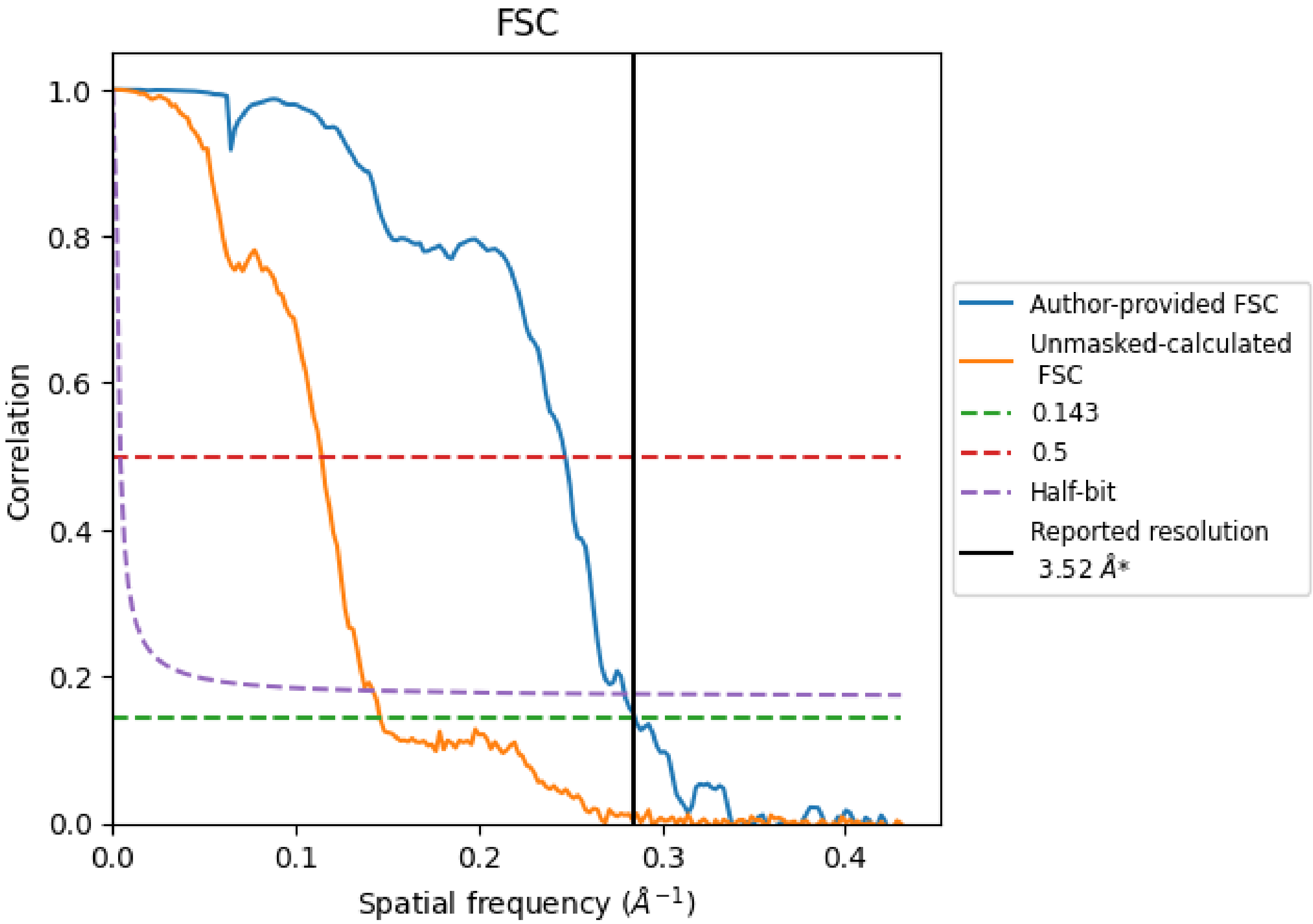


*Reported resolution corresponds to spatial frequency of 0.284 $\AA^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.284 $Å^{-1}$

8.2 Resolution estimates (i)

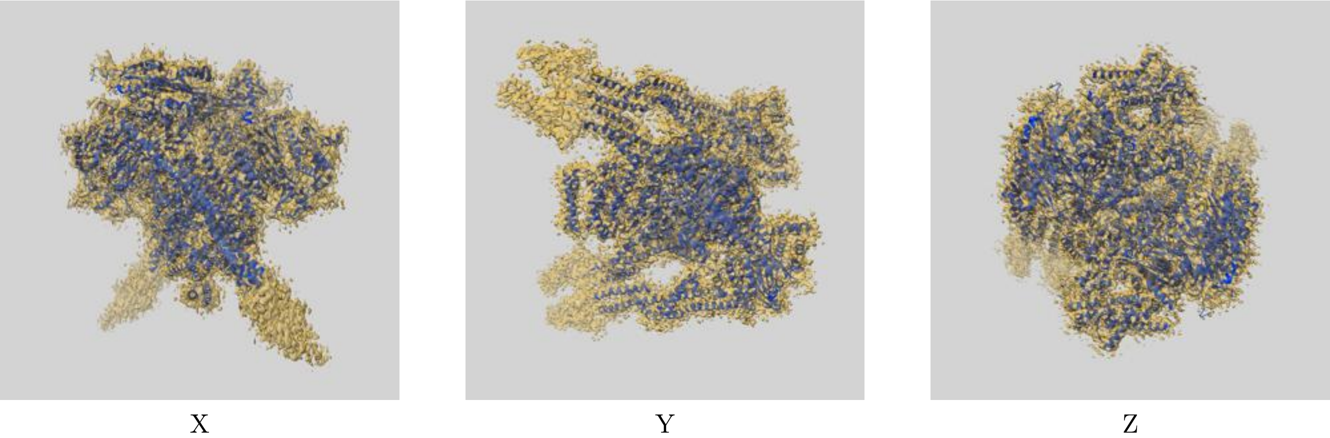
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.51	4.05	3.58
Unmasked-calculated*	6.84	8.76	7.03

*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 ⓘ

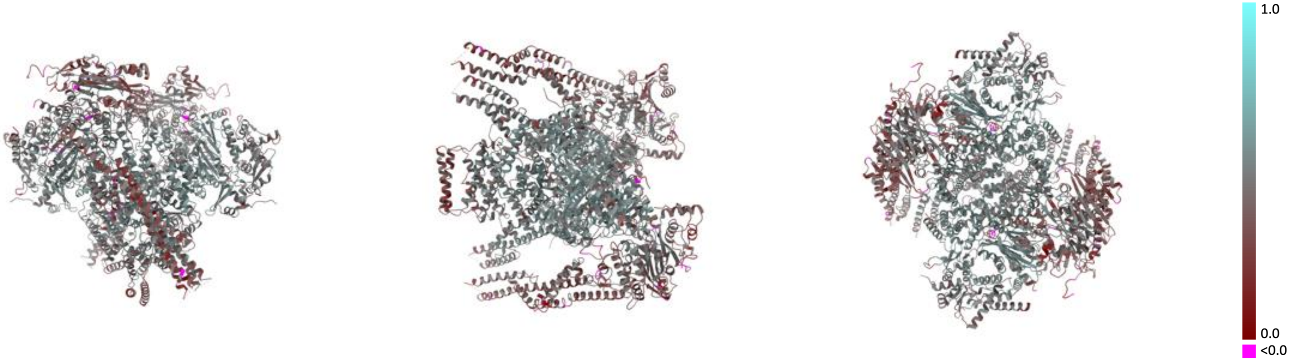
This section contains information regarding the fit between EMDB map EMD-16020 and PDB model 8BFN. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ



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.

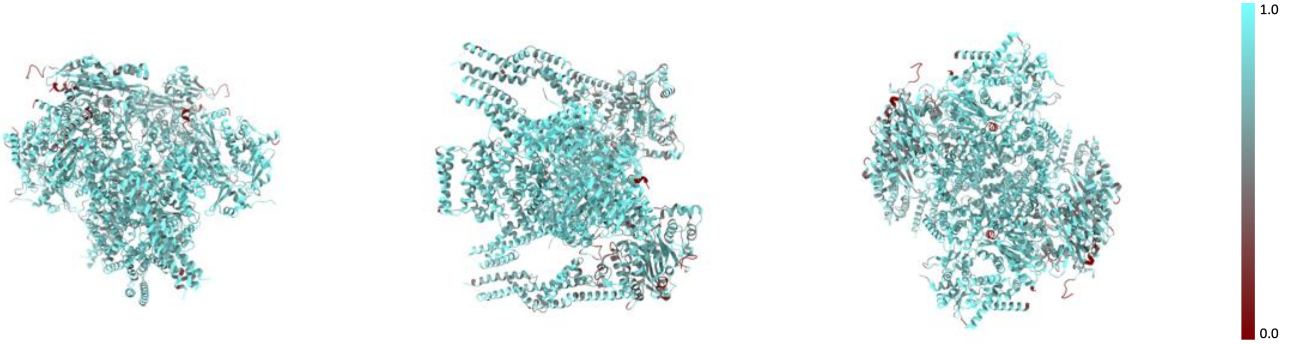
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

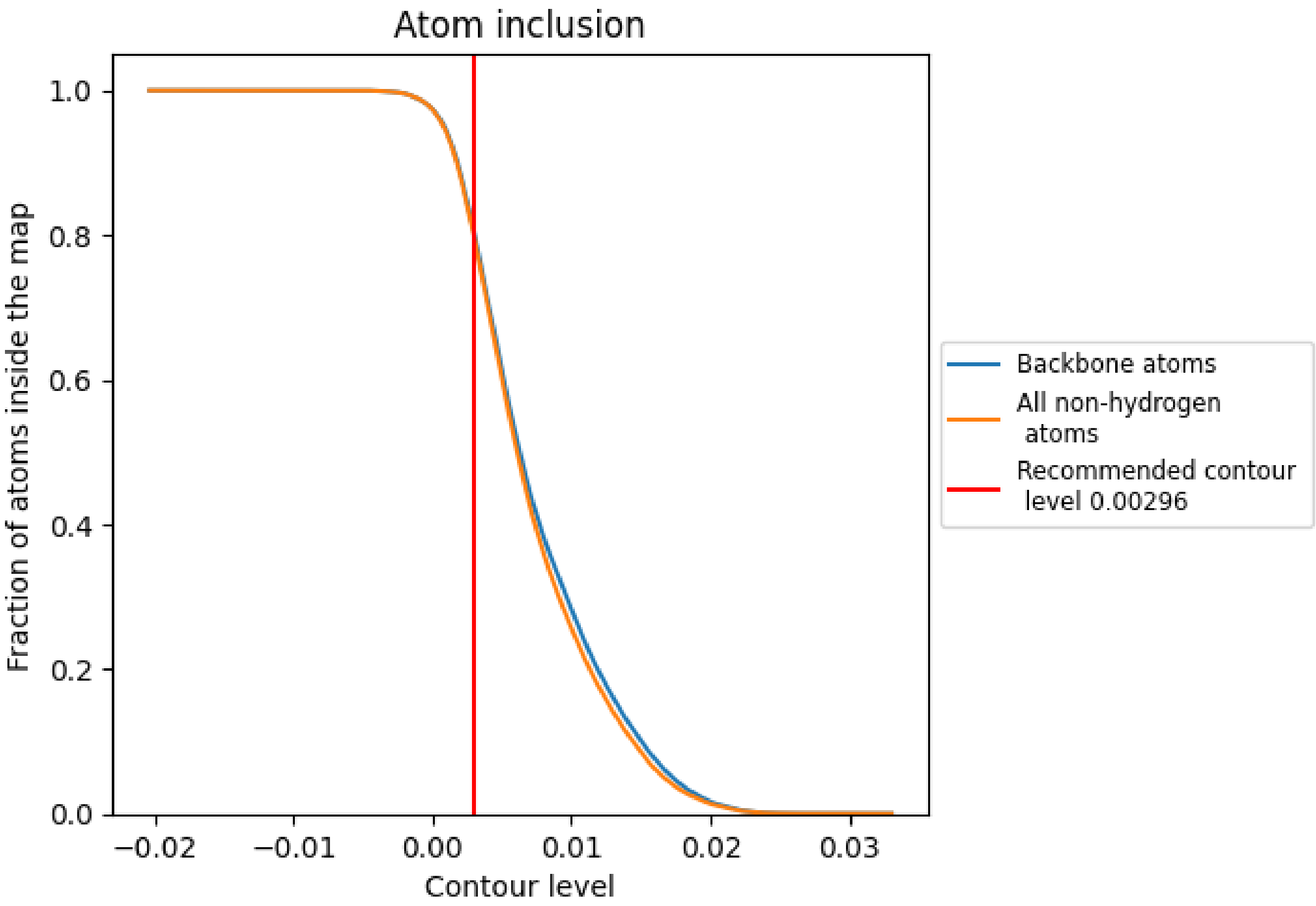
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



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 (i)

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	■ 0.8008	■ 0.4520
A	■ 0.8474	■ 0.5050
B	■ 0.7019	■ 0.3640
C	■ 0.8914	■ 0.5210
D	■ 0.8391	■ 0.4640
E	■ 0.8233	■ 0.4540
F	■ 0.8534	■ 0.5090
G	■ 0.7019	■ 0.3670
H	■ 0.8947	■ 0.5240
I	■ 0.8463	■ 0.4680
J	■ 0.8268	■ 0.4580