



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1GQ2
Title : MALIC ENZYME FROM PIGEON LIVER
Authors : Yang, Z.; Zhang, H.; Liang, T.
Deposited on : 2001-11-19
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

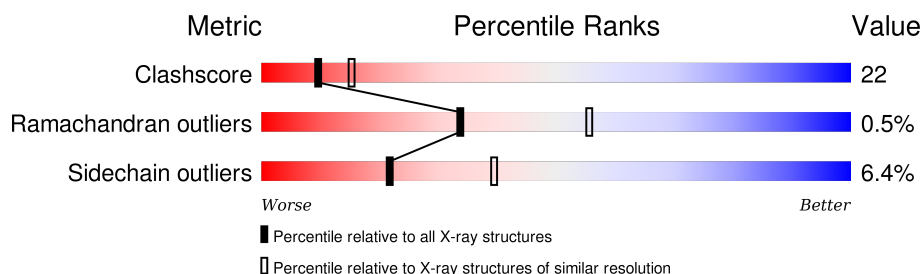
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)










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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	
1	C	555	
1	D	555	
1	E	555	
1	F	555	
1	G	555	

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Mol	Chain	Length	Quality of chain	
1	H	555		•
1	I	555		•
1	J	555		•
1	K	555		•
1	L	555		•
1	M	555		•
1	N	555		•
1	O	555		•
1	P	555		•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	C	1582	-	-	X	-
3	OXL	D	1582	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 71519 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	C	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	D	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	E	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	F	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	G	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	H	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	I	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	J	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	K	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	L	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	M	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	N	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	O	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	P	555	Total	C	N	O	S	Se	0	0	0
			4346	2772	742	807	11	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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C	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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E	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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F	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
G	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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G	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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H	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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I	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
J	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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J	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
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J	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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K	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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L	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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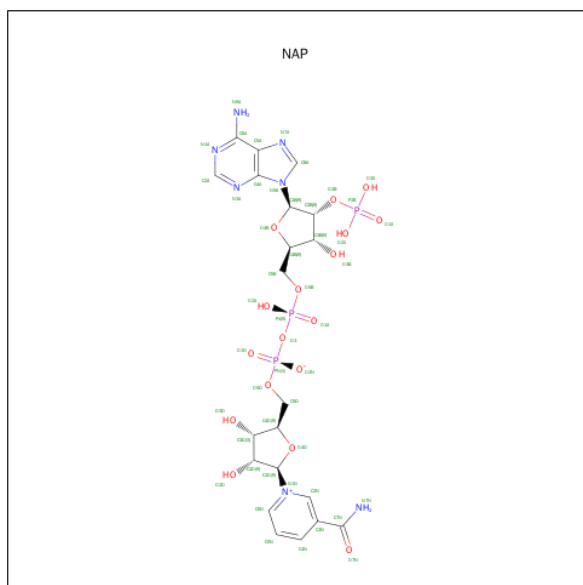
Chain	Residue	Modelled	Actual	Comment	Reference
M	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
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M	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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N	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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O	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
P	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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P	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



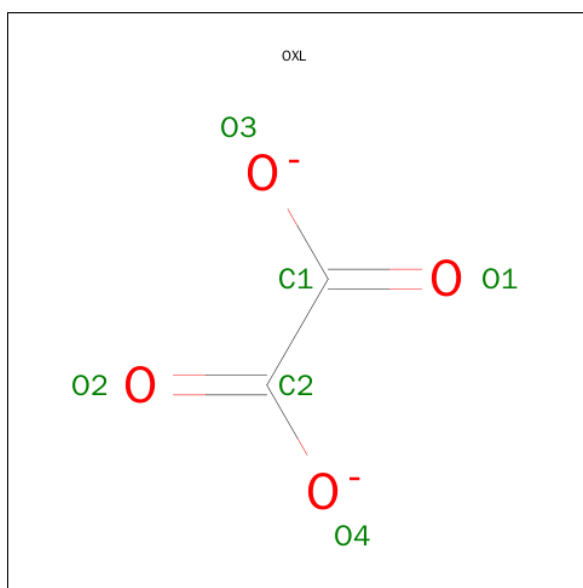
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0
3	I	1	Total C O 6 2 4	0	0
3	J	1	Total C O 6 2 4	0	0
3	K	1	Total C O 6 2 4	0	0
3	L	1	Total C O 6 2 4	0	0
3	M	1	Total C O 6 2 4	0	0
3	N	1	Total C O 6 2 4	0	0
3	O	1	Total C O 6 2 4	0	0
3	P	1	Total C O 6 2 4	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Mn 1 1	0	0
4	G	1	Total Mn 1 1	0	0
4	J	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total 1	Mn 1	0	0
4	E	1	Total 1	Mn 1	0	0
4	H	1	Total 1	Mn 1	0	0
4	B	1	Total 1	Mn 1	0	0
4	I	1	Total 1	Mn 1	0	0
4	C	1	Total 1	Mn 1	0	0
4	A	1	Total 1	Mn 1	0	0
4	N	1	Total 1	Mn 1	0	0
4	O	1	Total 1	Mn 1	0	0
4	L	1	Total 1	Mn 1	0	0
4	F	1	Total 1	Mn 1	0	0
4	M	1	Total 1	Mn 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	3	Total 3	Cl 3	0	0
5	G	1	Total 1	Cl 1	0	0
5	J	2	Total 2	Cl 2	0	0
5	K	1	Total 1	Cl 1	0	0
5	E	3	Total 3	Cl 3	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	5	Total 5	Cl 5	0	0
5	C	4	Total 4	Cl 4	0	0
5	N	2	Total 2	Cl 2	0	0
5	O	4	Total 4	Cl 4	0	0
5	L	1	Total 1	Cl 1	0	0
5	F	2	Total 2	Cl 2	0	0
5	M	3	Total 3	Cl 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	5	Total 5	Na 5	0	0
6	G	1	Total 1	Na 1	0	0
6	J	2	Total 2	Na 2	0	0
6	D	2	Total 2	Na 2	0	0
6	K	1	Total 1	Na 1	0	0
6	H	5	Total 5	Na 5	0	0
6	I	2	Total 2	Na 2	0	0
6	C	4	Total 4	Na 4	0	0
6	N	1	Total 1	Na 1	0	0
6	O	4	Total 4	Na 4	0	0
6	L	1	Total 1	Na 1	0	0
6	F	2	Total 2	Na 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	6	Total	Na	0	0
			6	6		

- Molecule 7 is water.

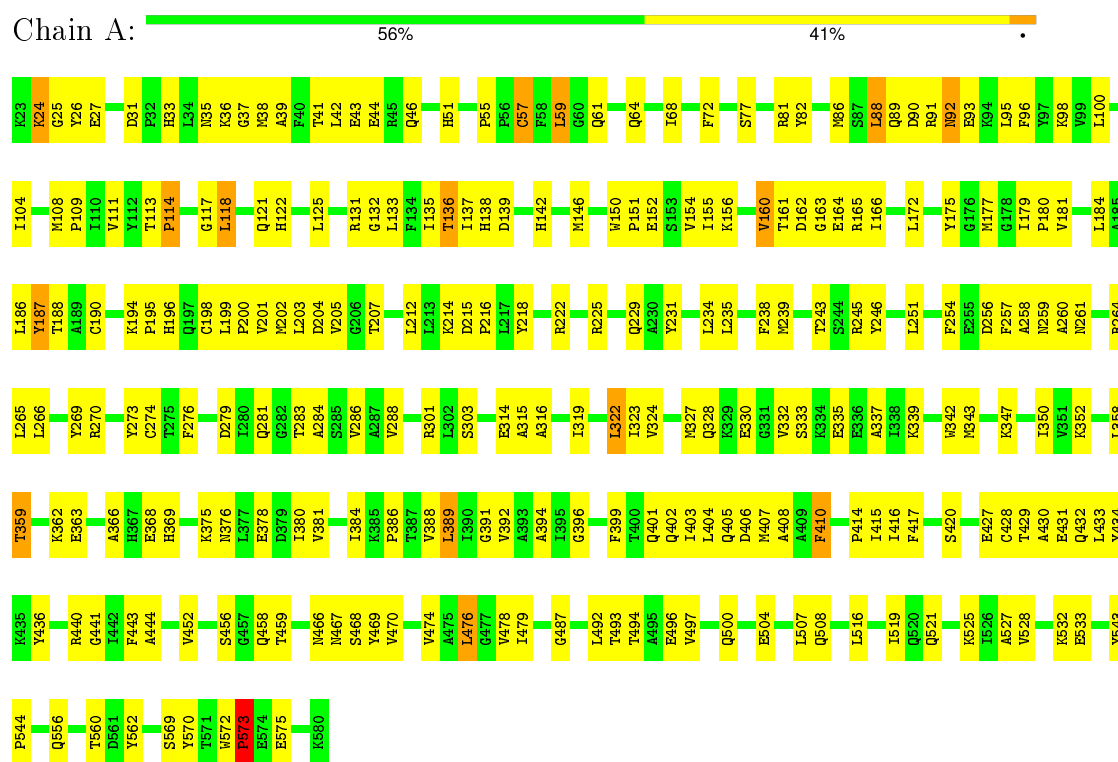
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	B	42	Total	O	0	0
			42	42		
7	C	77	Total	O	0	0
			77	77		
7	D	49	Total	O	0	0
			49	49		
7	E	58	Total	O	0	0
			58	58		
7	F	78	Total	O	0	0
			78	78		
7	G	65	Total	O	0	0
			65	65		
7	H	77	Total	O	0	0
			77	77		
7	I	80	Total	O	0	0
			80	80		
7	J	63	Total	O	0	0
			63	63		
7	K	41	Total	O	0	0
			41	41		
7	L	75	Total	O	0	0
			75	75		
7	M	81	Total	O	0	0
			81	81		
7	N	71	Total	O	0	0
			71	71		
7	O	78	Total	O	0	0
			78	78		
7	P	79	Total	O	0	0
			79	79		

3 Residue-property plots

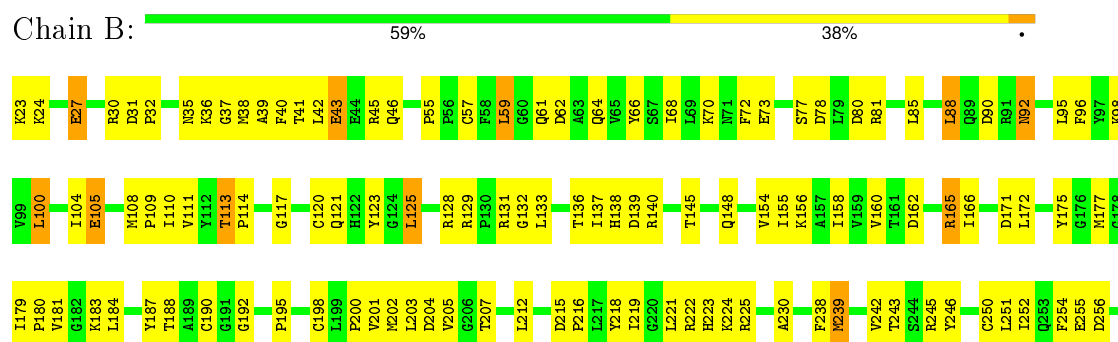
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

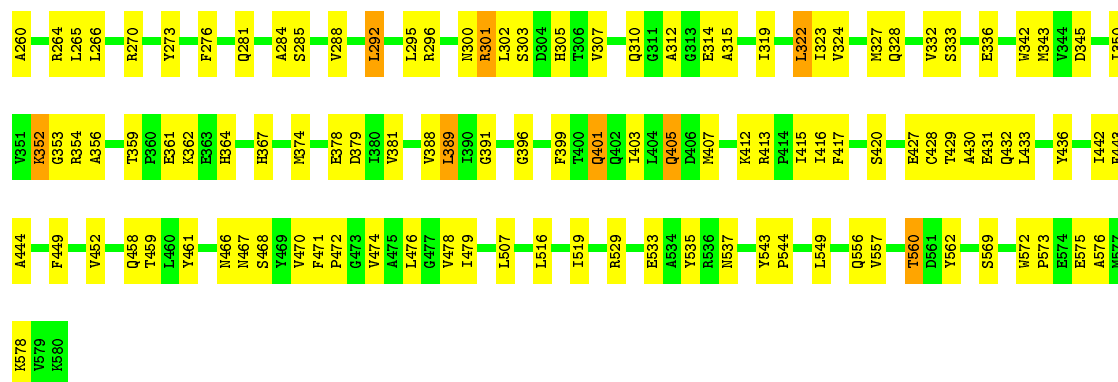
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



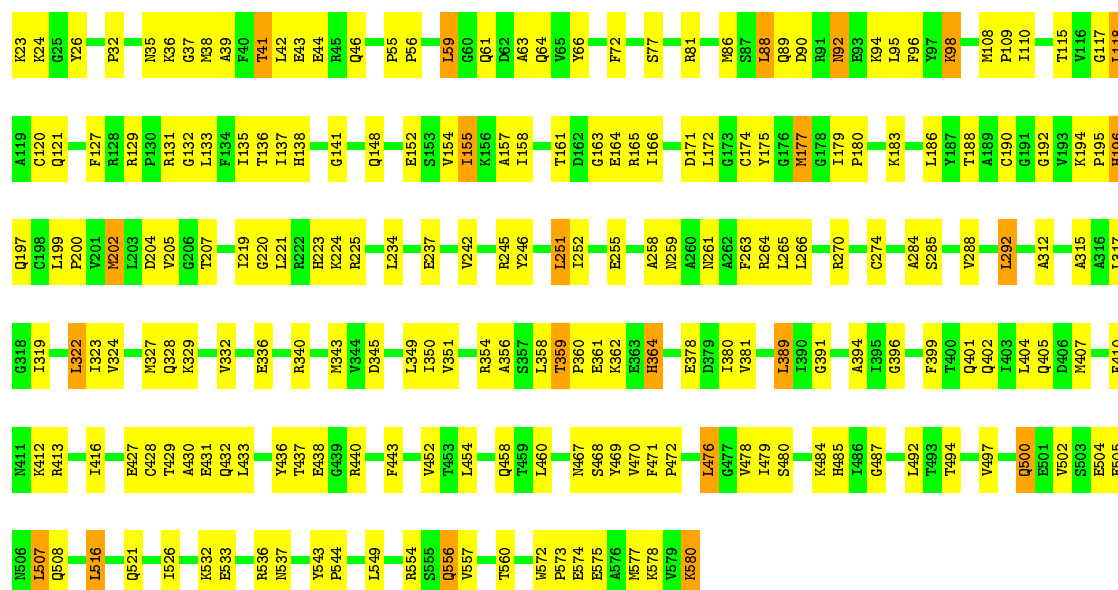
• Molecule 1: MALIC ENZYME





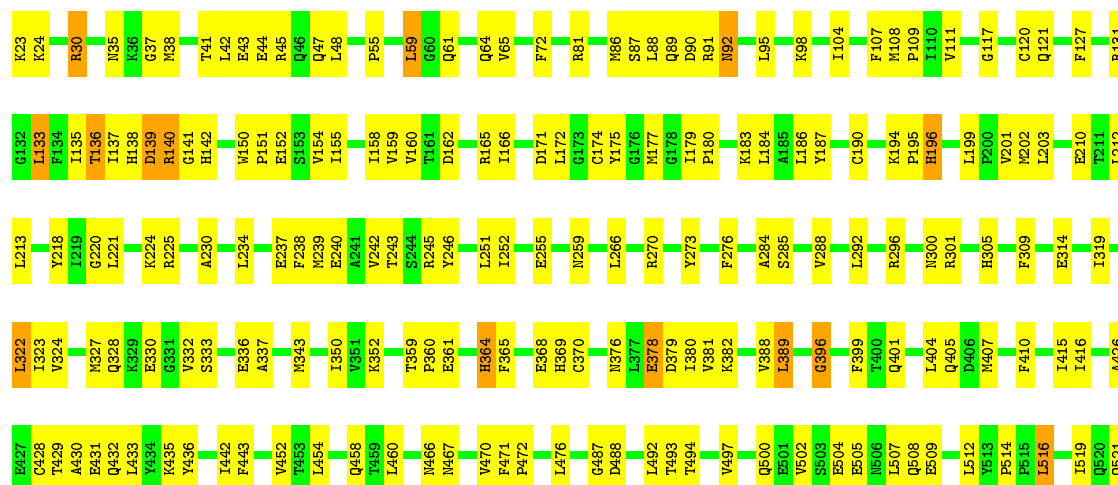
• Molecule 1: MALIC ENZYME

Chain C: 62% 34%



• Molecule 1: MALIC ENZYME

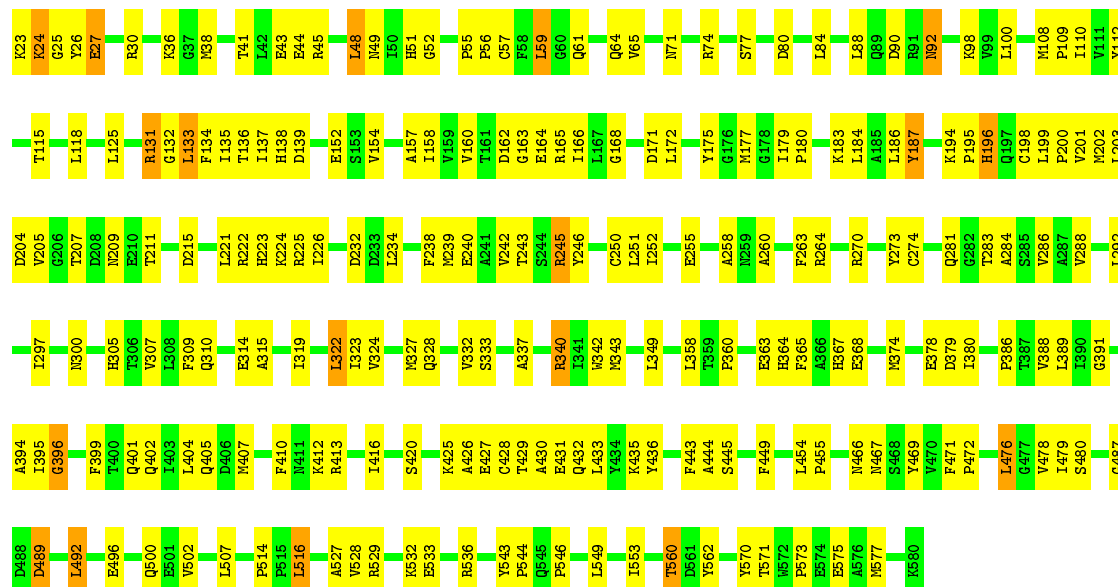
Chain D: 61% 35%





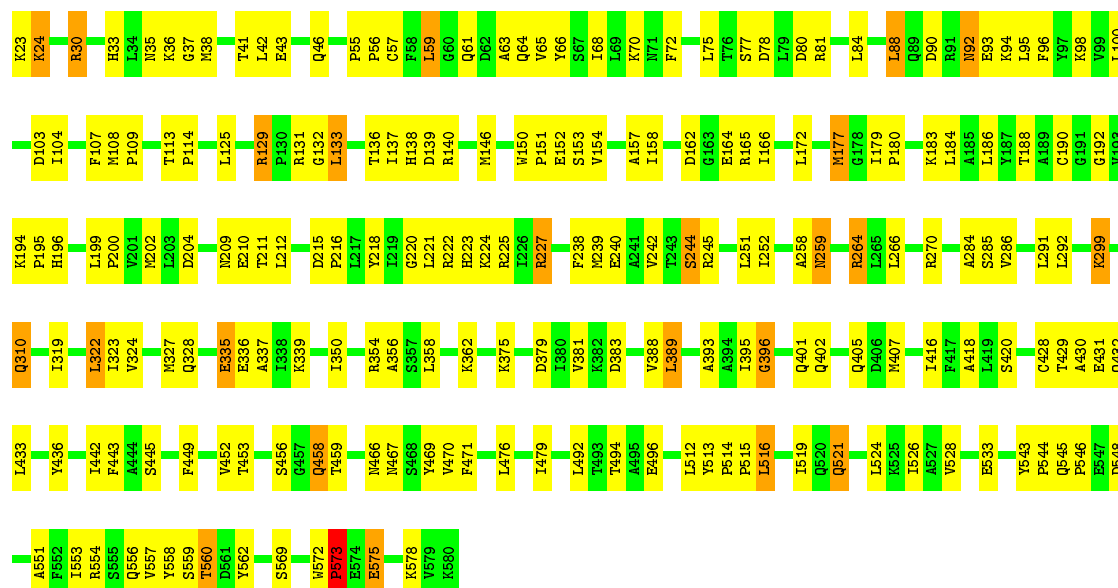
• Molecule 1: MALIC ENZYME

Chain E: 60% 36%



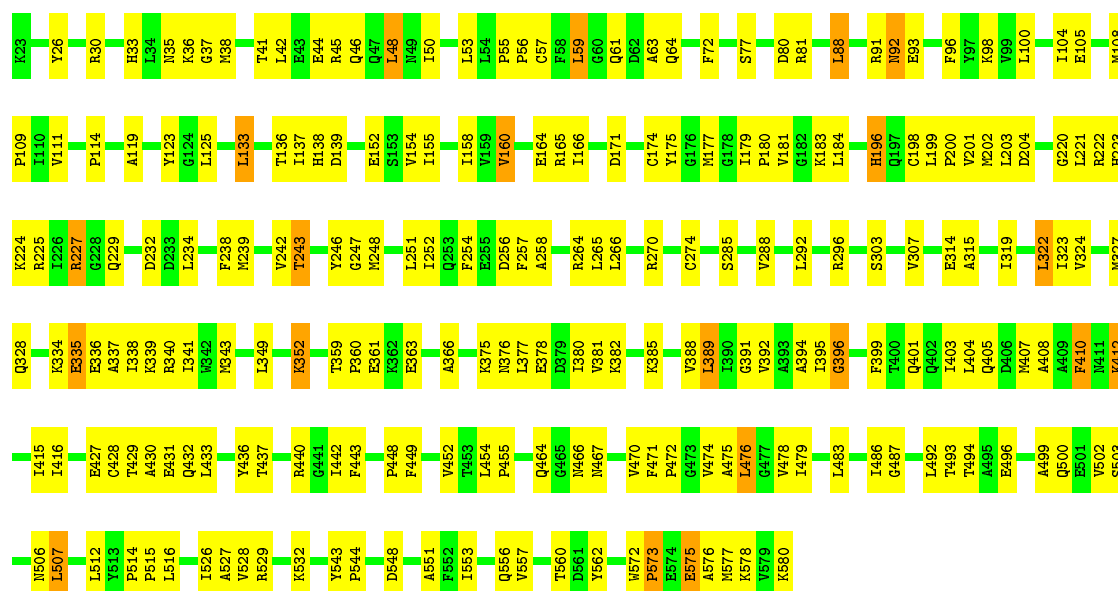
• Molecule 1: MALIC ENZYME

Chain F: 63% 33%

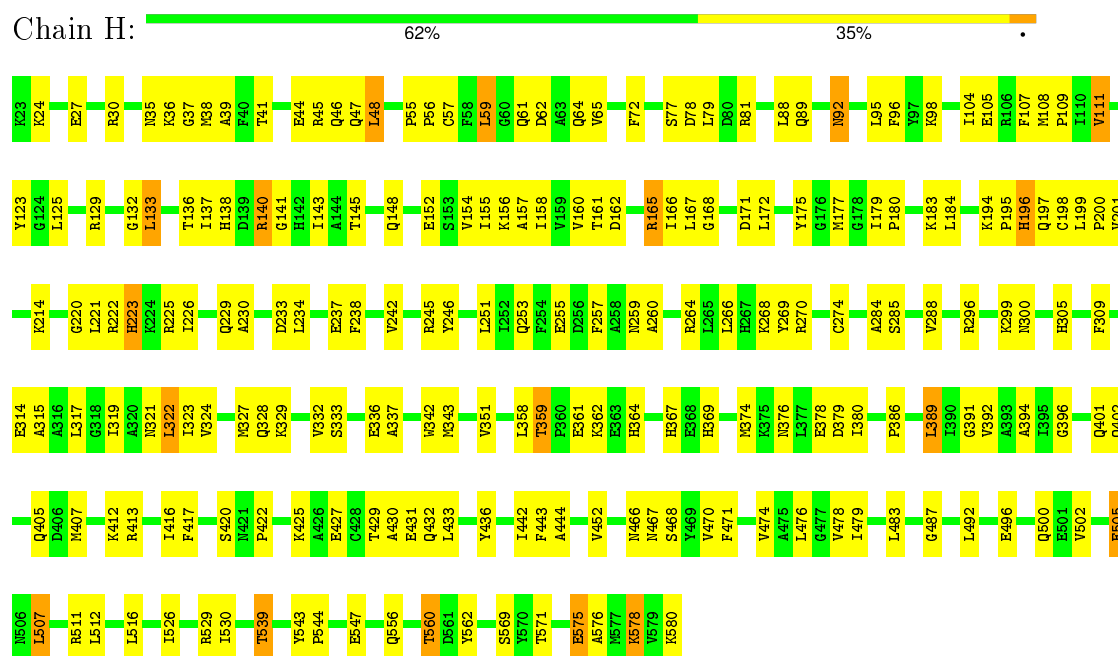


• Molecule 1: MALIC ENZYME

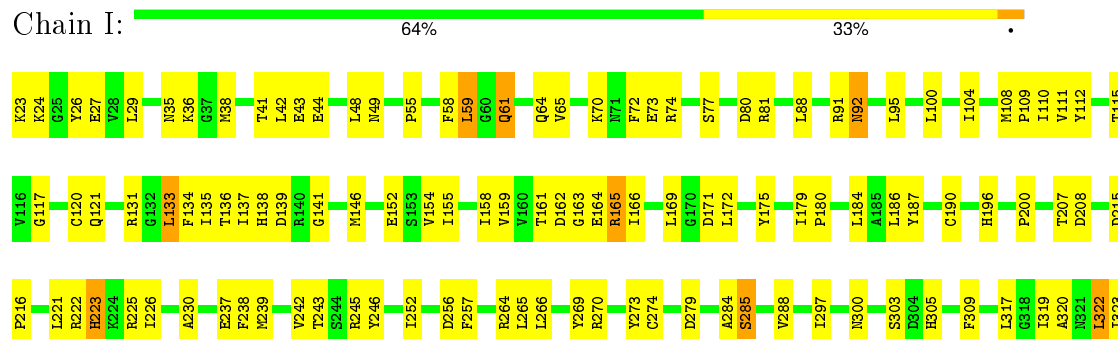
Chain G: 60% 36%

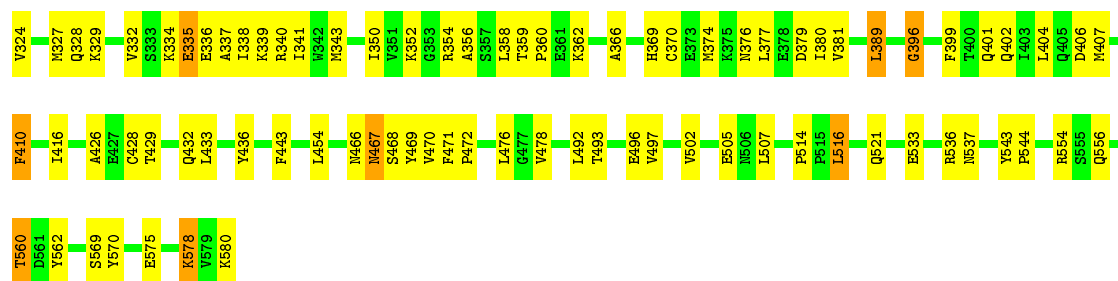


• Molecule 1: MALIC ENZYME



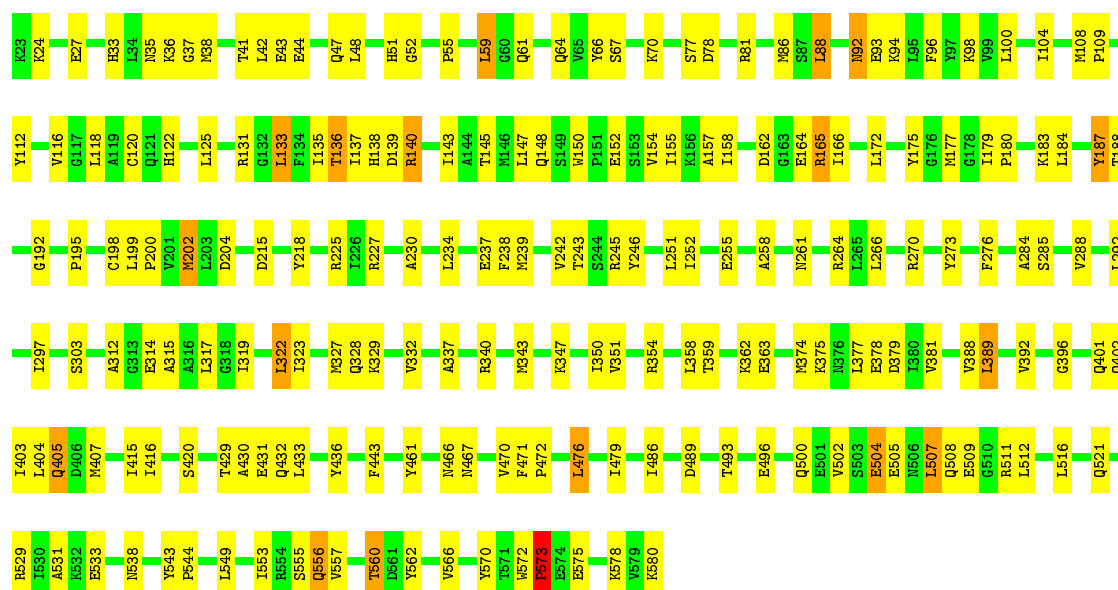
• Molecule 1: MALIC ENZYME





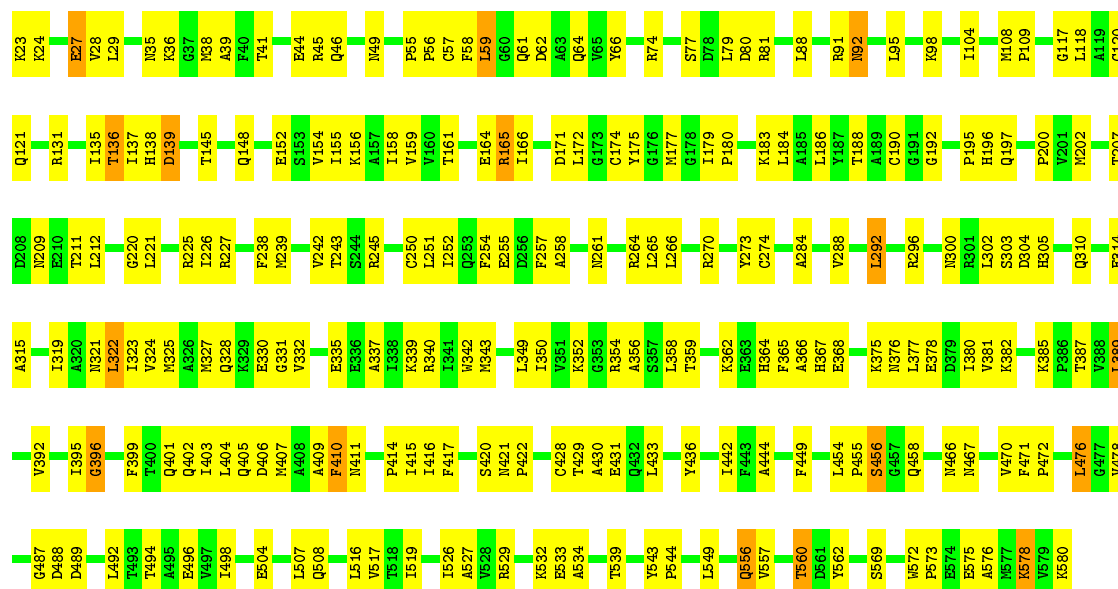
• Molecule 1: MALIC ENZYME

Chain J: 64% 33% .



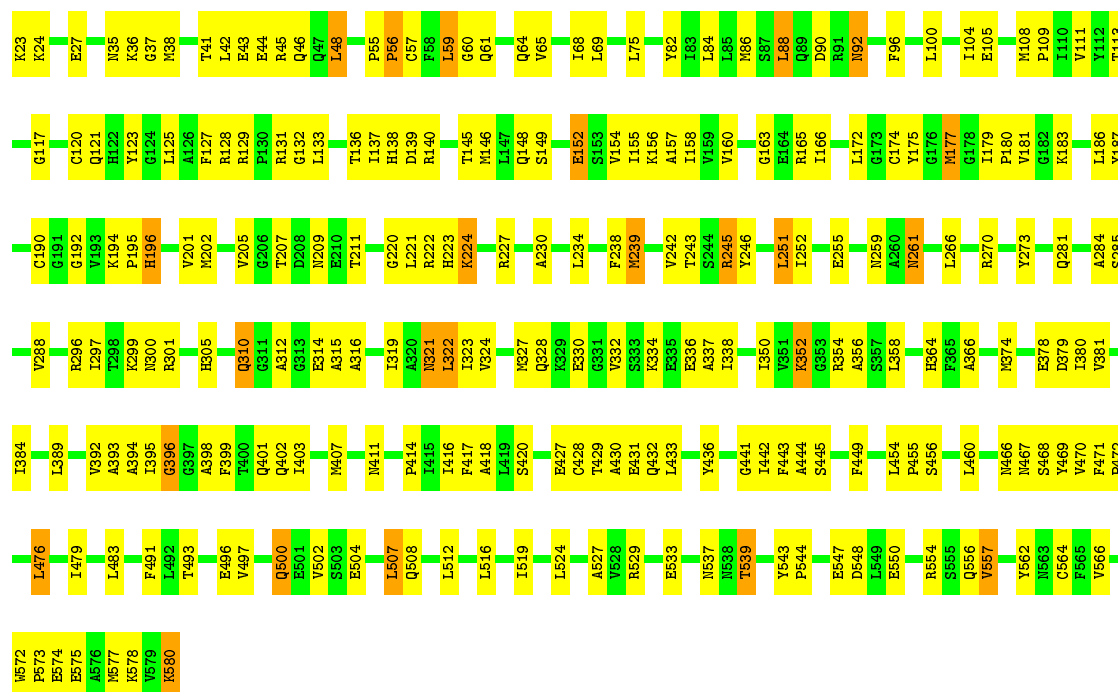
• Molecule 1: MALIC ENZYME

Chain K: 58% 39% .



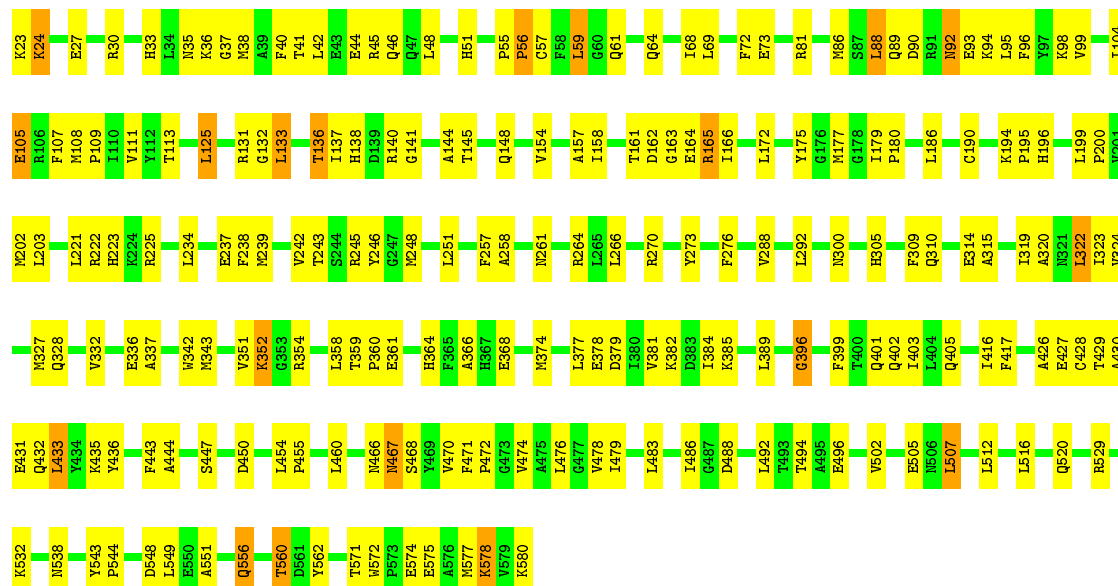
- Molecule 1: MALIC ENZYME

Chain L: 



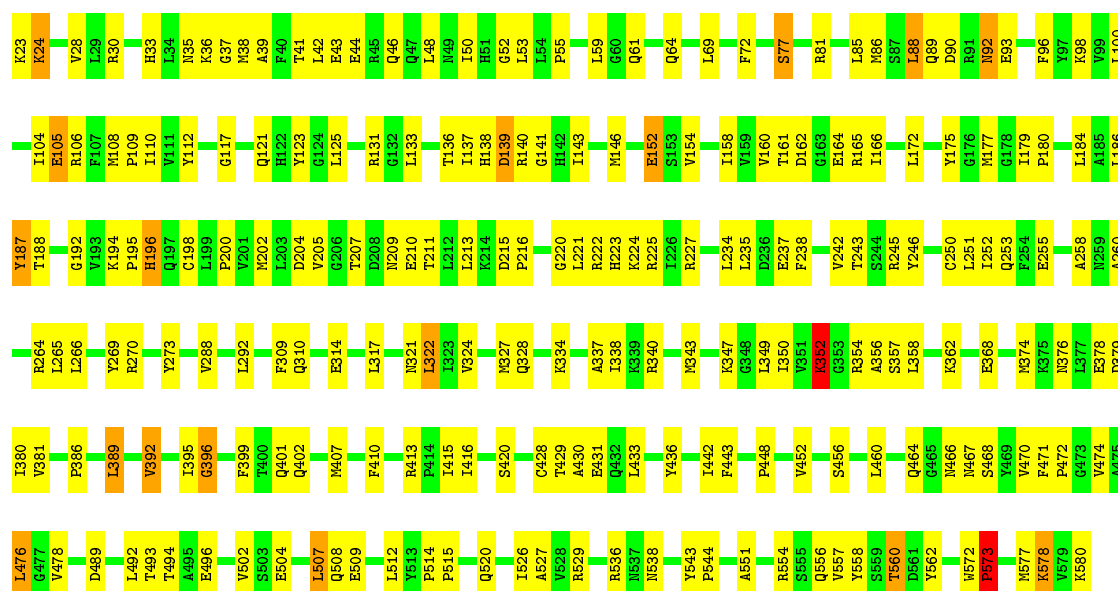
- Molecule 1: MALIC ENZYME

Chain M: 



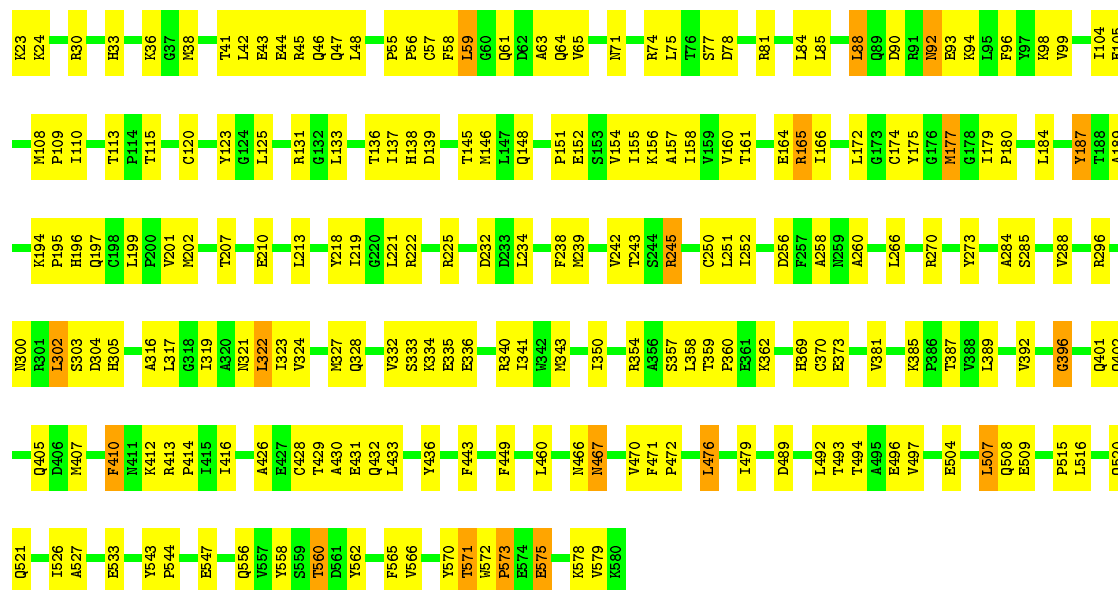
- Molecule 1: MALIC ENZYME

Chain N: 



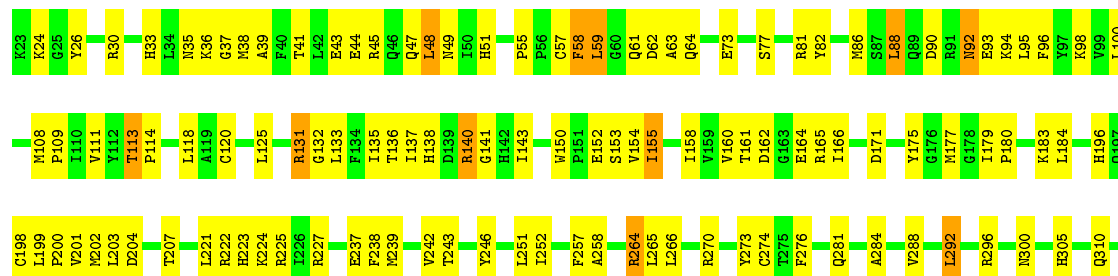
• Molecule 1: MALIC ENZYME

Chain O: 62% 35%



• Molecule 1: MALIC ENZYME

Chain P: 64% 32%



P544	T429	I319
R554	A430	L322
S555	E431	I323
Q556	Q432	M327
V557	L433	V332
Y558	E438	E336
S559	F443	A337
T560	L454	R340
D561	P455	I341
Y562	L460	V342
V566	M466	I350
W572	M467	L358
P573	S468	K362
E574	F471	E363
E575	G473	H364
K578	L476	E367
V579	G477	K374
K580	V478	K375
	G487	K376
	L492	D379
	T493	I380
	E496	V381
	V497	K385
	Q500	V388
	E501	L389
	V502	G396
	S503	F399
	E504	T400
	L507	Q401
	Q508	Q402
	L516	L403
	I519	L404
	Q520	Q405
	Q521	P406
	L524	M407
	V527	F410
	V528	M411
	R529	I415
	I530	I416
	E533	A426
	Y542	E432

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.15Å 140.86Å 167.08Å 90.05° 87.16° 75.63°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	71519	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, NA, NAP, MN, CL

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	0.39	0/4420	0.61	0/5962
1	B	0.38	0/4420	0.61	0/5962
1	C	0.40	0/4420	0.62	1/5962 (0.0%)
1	D	0.40	0/4420	0.62	0/5962
1	E	0.38	0/4420	0.61	0/5962
1	F	0.40	0/4420	0.63	1/5962 (0.0%)
1	G	0.39	0/4420	0.62	0/5962
1	H	0.41	0/4420	0.62	0/5962
1	I	0.40	0/4420	0.63	0/5962
1	J	0.40	0/4420	0.61	0/5962
1	K	0.39	0/4420	0.61	0/5962
1	L	0.39	0/4420	0.62	0/5962
1	M	0.41	0/4420	0.63	0/5962
1	N	0.40	0/4420	0.63	1/5962 (0.0%)
1	O	0.39	0/4420	0.62	0/5962
1	P	0.39	0/4421	0.62	0/5962
All	All	0.39	0/70721	0.62	3/95392 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	310	GLN	N-CA-C	-5.11	97.21	111.00
1	N	352	LYS	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4345	0	4366	230	0
1	B	4345	0	4366	216	0
1	C	4345	0	4366	219	0
1	D	4345	0	4366	196	0
1	E	4345	0	4366	189	0
1	F	4345	0	4366	193	0
1	G	4345	0	4366	197	0
1	H	4345	0	4366	178	0
1	I	4345	0	4366	181	0
1	J	4345	0	4366	200	0
1	K	4345	0	4366	208	0
1	L	4345	0	4366	227	0
1	M	4345	0	4366	188	0
1	N	4345	0	4366	207	0
1	O	4345	0	4366	226	0
1	P	4346	0	4366	194	0
2	A	48	0	25	4	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	H	48	0	25	3	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
2	K	48	0	25	5	0
2	L	48	0	25	5	0
2	M	48	0	25	3	0
2	N	48	0	25	3	0
2	O	48	0	25	2	0
2	P	48	0	25	1	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
3	C	6	0	0	3	0
3	D	6	0	0	2	0
3	E	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
3	I	6	0	0	0	0
3	J	6	0	0	1	0
3	K	6	0	0	1	0
3	L	6	0	0	1	0
3	M	6	0	0	0	0
3	N	6	0	0	1	0
3	O	6	0	0	0	0
3	P	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	1	0
5	E	3	0	0	1	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	5	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	1	0
5	N	2	0	0	1	0
5	O	4	0	0	3	0
5	P	3	0	0	3	0
6	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	G	1	0	0	0	0
6	H	5	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	6	0	0	0	0
6	N	1	0	0	0	0
6	O	4	0	0	0	0
6	P	5	0	0	0	0
7	A	35	0	0	6	0
7	B	42	0	0	6	0
7	C	77	0	0	7	0
7	D	49	0	0	2	0
7	E	58	0	0	5	0
7	F	78	0	0	6	0
7	G	65	0	0	6	0
7	H	77	0	0	7	0
7	I	80	0	0	7	0
7	J	63	0	0	3	0
7	K	41	0	0	5	0
7	L	75	0	0	7	0
7	M	81	0	0	7	0
7	N	71	0	0	7	0
7	O	78	0	0	8	0
7	P	79	0	0	4	0
All	All	71519	0	70256	3151	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 22.

All (3151) 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:H:136:THR:HG22	1:H:138:HIS:H	1.08	1.17
1:N:136:THR:HG22	1:N:138:HIS:H	1.04	1.17
1:K:98:LYS:HD3	1:K:560:THR:HG21	1.30	1.14
1:F:136:THR:HG22	1:F:138:HIS:H	1.10	1.13
1:B:136:THR:HG22	1:B:138:HIS:H	1.06	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:VAL:HG13	1:N:407:MSE:HE2	1.30	1.13
1:G:416:ILE:HG13	1:G:433:LEU:HD21	1.24	1.13
1:M:429:THR:HB	1:M:432:GLN:HG3	1.34	1.10
1:E:136:THR:HG22	1:E:138:HIS:H	1.06	1.10
1:O:323:ILE:HG22	1:O:327:MSE:HE2	1.25	1.10
1:K:136:THR:HG23	1:K:138:HIS:H	1.08	1.10
1:P:136:THR:HG22	1:P:138:HIS:H	1.04	1.09
1:C:136:THR:HG22	1:C:138:HIS:H	1.08	1.09
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.33	1.08
1:C:494:THR:HG23	1:C:526:ILE:HD12	1.35	1.08
1:C:323:ILE:HG22	1:C:327:MSE:HE2	1.36	1.08
1:I:136:THR:HG22	1:I:138:HIS:H	1.09	1.08
1:D:160:VAL:HG12	1:D:201:VAL:HB	1.30	1.07
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.35	1.07
1:O:136:THR:HG22	1:O:138:HIS:H	1.12	1.07
1:A:386:PRO:HG2	1:A:407:MSE:HE1	1.13	1.07
1:L:136:THR:HG22	1:L:138:HIS:H	1.04	1.06
1:L:327:MSE:HE3	1:L:337:ALA:HB1	1.38	1.05
1:P:160:VAL:HG22	1:P:201:VAL:HB	1.40	1.04
1:K:327:MSE:HE3	1:K:337:ALA:HB1	1.39	1.04
1:M:136:THR:HG23	1:M:138:HIS:H	1.17	1.03
1:E:386:PRO:HG2	1:E:407:MSE:HE1	1.36	1.03
1:G:136:THR:HG22	1:G:138:HIS:H	1.24	1.03
1:J:136:THR:HG22	1:J:138:HIS:H	1.20	1.01
1:P:327:MSE:HE3	1:P:337:ALA:HB1	1.40	1.01
1:O:104:ILE:HG13	1:O:108:MSE:HE3	1.38	1.00
1:N:327:MSE:HE3	1:N:337:ALA:HB1	1.40	1.00
1:G:177:MSE:HE1	1:G:200:PRO:HB2	1.42	1.00
1:C:416:ILE:HG13	1:C:433:LEU:HD21	1.40	0.99
1:M:429:THR:H	1:M:432:GLN:HE21	1.04	0.98
1:B:416:ILE:HG13	1:B:433:LEU:HD21	1.39	0.98
1:N:36:LYS:HG2	1:N:39:ALA:HB3	1.45	0.98
1:E:24:LYS:HG2	1:E:25:GLY:N	1.77	0.97
1:H:327:MSE:HE3	1:H:337:ALA:HB1	1.44	0.97
1:E:24:LYS:HZ2	1:E:49:ASN:HD22	1.00	0.97
1:N:504:GLU:HG3	1:N:508:GLN:HE21	1.30	0.96
1:M:238:PHE:HD2	1:M:239:MSE:HE2	1.29	0.96
1:L:416:ILE:HG13	1:L:433:LEU:HD21	1.48	0.96
1:L:261:ASN:H	1:L:261:ASN:HD22	1.11	0.95
1:L:145:THR:O	1:L:148:GLN:HG2	1.65	0.95
1:H:359:THR:HG22	1:H:362:LYS:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:386:PRO:HG2	1:H:407:MSE:HE1	1.47	0.95
1:P:136:THR:HG22	1:P:138:HIS:N	1.81	0.94
1:F:177:MSE:HE3	1:F:177:MSE:HA	1.49	0.94
1:K:136:THR:HG23	1:K:138:HIS:N	1.81	0.94
1:J:136:THR:CG2	1:J:138:HIS:H	1.80	0.94
1:P:504:GLU:HG3	1:P:508:GLN:HE22	1.30	0.94
1:L:136:THR:HG22	1:L:138:HIS:N	1.82	0.94
1:P:416:ILE:HG13	1:P:433:LEU:HD21	1.49	0.94
1:D:547:GLU:H	1:D:547:GLU:CD	1.65	0.94
1:D:136:THR:HG23	1:D:138:HIS:H	1.31	0.94
1:P:36:LYS:HG2	1:P:39:ALA:HB3	1.50	0.93
1:E:24:LYS:HZ2	1:E:49:ASN:ND2	1.64	0.93
1:O:160:VAL:HG22	1:O:201:VAL:HB	1.51	0.93
1:L:261:ASN:HD22	1:L:261:ASN:N	1.67	0.93
1:I:429:THR:HG23	1:I:432:GLN:H	1.33	0.93
1:M:454:LEU:HD11	1:M:460:LEU:HG	1.51	0.93
1:E:327:MSE:HE3	1:E:337:ALA:HB1	1.50	0.92
1:A:41:THR:HB	1:A:44:GLU:HG3	1.51	0.92
1:G:378:GLU:HA	1:G:403:ILE:HD11	1.51	0.92
1:A:42:LEU:HD23	1:C:577:MSE:HE3	1.50	0.91
1:G:164:GLU:HG2	1:G:258:ALA:HB2	1.51	0.91
1:A:36:LYS:HG2	1:A:39:ALA:HB3	1.52	0.91
1:I:136:THR:HG22	1:I:138:HIS:N	1.85	0.91
1:C:23:LYS:HG2	1:C:24:LYS:H	1.34	0.91
1:O:401:GLN:HG2	1:O:405:GLN:HE21	1.33	0.91
1:B:98:LYS:HD3	1:B:560:THR:HG21	1.50	0.91
1:C:136:THR:HG22	1:C:138:HIS:N	1.87	0.90
1:F:429:THR:H	1:F:432:GLN:NE2	1.69	0.90
1:A:570:TYR:H	1:C:46:GLN:HE22	1.19	0.89
1:D:23:LYS:HG2	1:D:24:LYS:H	1.36	0.89
1:N:136:THR:HG22	1:N:138:HIS:N	1.87	0.89
1:K:416:ILE:HG13	1:K:433:LEU:HD21	1.53	0.89
1:B:140:ARG:HH12	1:B:230:ALA:HB1	1.38	0.89
1:N:389:LEU:HG	1:N:407:MSE:HE3	1.54	0.89
1:J:429:THR:HB	1:J:432:GLN:HG2	1.54	0.88
1:L:239:MSE:HA	1:L:239:MSE:HE2	1.55	0.88
1:O:136:THR:HB	1:O:139:ASP:OD2	1.73	0.88
1:O:412:LYS:HB2	1:O:412:LYS:NZ	1.88	0.88
1:E:136:THR:HG22	1:E:138:HIS:N	1.89	0.88
1:M:578:LYS:NZ	1:M:580:LYS:HB2	1.89	0.88
1:E:429:THR:HG22	1:E:431:GLU:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:ARG:HG3	1:G:222:ARG:HH11	1.39	0.88
1:N:98:LYS:HD3	1:N:560:THR:HG21	1.55	0.88
1:L:104:ILE:HG13	1:L:108:MSE:HE3	1.56	0.87
1:D:324:VAL:HG12	1:D:328:GLN:HE21	1.39	0.87
1:A:466:ASN:HA	2:A:1581:NAP:H72N	1.39	0.87
1:G:560:THR:HG23	7:G:2062:HOH:O	1.74	0.87
1:J:416:ILE:HG13	1:J:433:LEU:HD21	1.57	0.87
1:A:358:LEU:HD23	1:A:363:GLU:HG3	1.56	0.87
1:O:238:PHE:CD2	1:O:239:MSE:HE3	2.09	0.87
1:E:98:LYS:HD3	1:E:560:THR:HG21	1.56	0.87
1:B:239:MSE:HE1	1:B:252:ILE:HG12	1.56	0.86
1:A:238:PHE:HD2	1:A:239:MSE:HE2	1.38	0.86
1:L:429:THR:HB	1:L:432:GLN:HG3	1.57	0.86
1:P:136:THR:CG2	1:P:138:HIS:H	1.87	0.86
1:J:466:ASN:HA	2:J:1581:NAP:H72N	1.38	0.86
1:G:136:THR:HG22	1:G:138:HIS:N	1.91	0.86
1:F:572:TRP:O	1:F:573:PRO:O	1.94	0.86
1:A:569:SER:HA	1:C:46:GLN:NE2	1.91	0.86
1:H:575:GLU:O	1:H:578:LYS:HG2	1.73	0.86
1:P:143:ILE:HD12	1:P:237:GLU:HG2	1.58	0.85
1:J:136:THR:HG22	1:J:138:HIS:N	1.90	0.85
1:K:239:MSE:HA	1:K:239:MSE:HE2	1.56	0.85
1:C:36:LYS:HG2	1:C:39:ALA:HB3	1.56	0.85
1:N:416:ILE:HG13	1:N:433:LEU:HD21	1.57	0.85
1:G:575:GLU:HG2	1:G:576:ALA:N	1.88	0.85
1:M:433:LEU:HG	1:M:443:PHE:HB2	1.59	0.85
1:A:572:TRP:O	1:A:573:PRO:O	1.94	0.85
1:B:239:MSE:HE2	1:B:239:MSE:HA	1.56	0.85
1:G:429:THR:H	1:G:432:GLN:NE2	1.75	0.85
1:I:327:MSE:HE3	1:I:337:ALA:HB1	1.55	0.85
1:O:239:MSE:HA	1:O:239:MSE:HE2	1.59	0.84
1:O:41:THR:HB	1:O:44:GLU:HG3	1.58	0.84
1:I:133:LEU:HD22	1:I:135:ILE:HG13	1.58	0.84
1:A:136:THR:CG2	1:A:138:HIS:H	1.91	0.84
1:M:327:MSE:HE3	1:M:337:ALA:HB1	1.59	0.84
1:N:24:LYS:HG2	1:P:24:LYS:NZ	1.93	0.84
1:M:24:LYS:HB2	1:M:24:LYS:NZ	1.89	0.84
1:H:416:ILE:HG13	1:H:433:LEU:HD21	1.57	0.84
1:M:401:GLN:O	1:M:405:GLN:HG3	1.77	0.84
1:B:136:THR:HB	1:B:139:ASP:OD1	1.78	0.83
1:J:572:TRP:O	1:J:573:PRO:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:VAL:CG1	1:N:407:MSE:HE2	2.07	0.83
1:F:129:ARG:HG3	1:F:129:ARG:HH11	1.42	0.83
1:J:327:MSE:HE3	1:J:337:ALA:HB1	1.57	0.83
1:E:340:ARG:HH11	1:E:340:ARG:HB3	1.44	0.83
1:B:41:THR:HG22	1:B:43:GLU:H	1.43	0.83
1:B:352:LYS:HE2	1:B:353:GLY:H	1.42	0.83
1:G:378:GLU:HA	1:G:403:ILE:CD1	2.09	0.83
1:K:152:GLU:OE2	1:K:154:VAL:HG12	1.78	0.83
7:N:2067:HOH:O	1:O:222:ARG:HD2	1.77	0.83
1:A:359:THR:HG22	1:A:362:LYS:HE2	1.61	0.83
1:D:35:ASN:ND2	1:D:37:GLY:H	1.77	0.83
1:J:98:LYS:HD3	1:J:560:THR:HG21	1.60	0.83
1:K:164:GLU:HG2	1:K:258:ALA:HB2	1.60	0.83
1:L:132:GLY:HA3	1:L:177:MSE:HE1	1.58	0.83
1:G:324:VAL:HG12	1:G:328:GLN:HE21	1.43	0.83
1:B:301:ARG:NH1	1:B:301:ARG:HB3	1.94	0.82
1:J:578:LYS:HE2	1:J:580:LYS:HE3	1.61	0.82
1:A:316:ALA:HB1	1:A:343:MSE:CE	2.10	0.82
1:L:136:THR:CG2	1:L:138:HIS:H	1.90	0.82
1:F:238:PHE:CD2	1:F:239:MSE:HE3	2.14	0.82
1:I:136:THR:CG2	1:I:138:HIS:H	1.93	0.82
1:D:238:PHE:CD2	1:D:239:MSE:HE2	2.15	0.82
1:D:23:LYS:HG2	1:D:24:LYS:N	1.92	0.82
1:D:359:THR:HG22	1:D:361:GLU:H	1.44	0.82
1:J:238:PHE:CD2	1:J:239:MSE:HE2	2.15	0.82
1:F:239:MSE:HE2	1:F:239:MSE:HA	1.61	0.81
1:O:59:LEU:HD13	1:O:64:GLN:HG3	1.61	0.81
1:I:350:ILE:HG23	1:I:358:LEU:HD11	1.60	0.81
1:F:433:LEU:HG	1:F:443:PHE:CD1	2.15	0.81
1:A:26:TYR:HB2	7:A:2002:HOH:O	1.79	0.81
1:J:359:THR:HG23	1:J:362:LYS:H	1.43	0.81
1:B:136:THR:HG22	1:B:138:HIS:N	1.92	0.81
1:L:466:ASN:HA	2:L:1581:NAP:H72N	1.44	0.81
1:F:88:LEU:HD21	1:F:95:LEU:HD12	1.62	0.81
1:O:429:THR:HB	1:O:432:GLN:HG2	1.63	0.81
1:D:136:THR:HG23	1:D:138:HIS:N	1.96	0.81
1:L:35:ASN:ND2	1:L:37:GLY:H	1.79	0.81
1:L:381:VAL:CG1	1:L:407:MSE:HE1	2.11	0.81
1:P:504:GLU:HG3	1:P:508:GLN:NE2	1.95	0.81
1:I:429:THR:HG22	1:I:432:GLN:CG	2.10	0.81
1:F:136:THR:HG23	1:F:221:LEU:HD11	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:LYS:HD3	1:K:560:THR:CG2	2.11	0.80
1:H:154:VAL:HG12	7:H:2026:HOH:O	1.81	0.80
1:B:98:LYS:HD3	1:B:560:THR:CG2	2.11	0.80
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.63	0.80
1:O:23:LYS:O	1:O:24:LYS:HG3	1.81	0.80
1:H:288:VAL:HG21	1:H:322:LEU:HB3	1.64	0.80
1:N:386:PRO:HG2	1:N:407:MSE:HE1	1.62	0.80
1:N:340:ARG:HD3	7:N:2043:HOH:O	1.81	0.80
1:A:98:LYS:HD3	1:A:560:THR:HG21	1.61	0.80
1:M:24:LYS:HD2	1:O:24:LYS:HZ2	1.47	0.80
1:K:36:LYS:HG2	1:K:39:ALA:HB3	1.64	0.80
1:D:133:LEU:HD13	1:D:135:ILE:HD11	1.63	0.80
1:O:177:MSE:CE	1:O:177:MSE:HA	2.12	0.79
1:F:136:THR:HG22	1:F:138:HIS:N	1.94	0.79
1:M:104:ILE:HG13	1:M:108:MSE:HE3	1.63	0.79
1:P:41:THR:HG22	1:P:43:GLU:H	1.47	0.79
1:D:41:THR:HG22	1:D:43:GLU:H	1.45	0.79
1:H:92:ASN:C	1:H:92:ASN:HD22	1.85	0.79
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.13	0.79
1:O:136:THR:HG23	1:O:221:LEU:HD11	1.63	0.79
1:F:416:ILE:HG13	1:F:433:LEU:HD21	1.63	0.79
1:J:104:ILE:HG13	1:J:108:MSE:HE3	1.65	0.79
1:D:416:ILE:HG13	1:D:433:LEU:HD21	1.65	0.78
1:K:415:ILE:CD1	1:K:442:ILE:HD12	2.14	0.78
1:K:238:PHE:CD2	1:K:239:MSE:HE3	2.19	0.78
1:H:136:THR:HG22	1:H:138:HIS:N	1.92	0.78
1:O:328:GLN:NE2	1:O:334:LYS:HD2	1.98	0.78
1:N:572:TRP:O	1:N:573:PRO:O	2.02	0.78
1:G:136:THR:CG2	1:G:138:HIS:H	1.94	0.78
1:M:92:ASN:HD22	1:M:92:ASN:C	1.85	0.78
1:H:378:GLU:OE2	1:H:402:GLN:HB3	1.84	0.78
1:O:433:LEU:HD12	1:O:443:PHE:HB2	1.64	0.78
1:I:41:THR:HB	1:I:44:GLU:HG3	1.66	0.77
1:D:572:TRP:O	1:D:573:PRO:O	2.02	0.77
1:H:36:LYS:HG2	1:H:39:ALA:HB3	1.65	0.77
1:O:136:THR:HG22	1:O:138:HIS:N	1.96	0.77
1:H:575:GLU:HG2	1:H:576:ALA:N	1.97	0.77
1:G:396:GLY:HA3	7:G:2041:HOH:O	1.84	0.77
1:J:225:ARG:HB2	1:J:227:ARG:NH1	2.00	0.77
1:E:160:VAL:HG12	1:E:201:VAL:HB	1.65	0.77
1:F:299:LYS:HB3	1:F:299:LYS:NZ	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:PHE:HD2	1:D:239:MSE:HE2	1.49	0.77
1:G:137:ILE:HA	1:G:234:LEU:HD22	1.66	0.77
1:E:239:MSE:HE2	1:E:239:MSE:HA	1.65	0.77
1:I:238:PHE:CD2	1:I:239:MSE:HE3	2.20	0.77
1:N:104:ILE:HG12	1:N:108:MSE:HE3	1.67	0.76
1:N:324:VAL:HG12	1:N:328:GLN:HE21	1.49	0.76
1:M:416:ILE:HB	1:M:433:LEU:HD21	1.68	0.76
1:C:38:MSE:HB2	1:C:59:LEU:HD11	1.67	0.76
1:O:47:GLN:HE22	1:O:566:VAL:HG13	1.49	0.76
1:G:177:MSE:HE3	1:G:181:VAL:HG23	1.68	0.76
1:E:238:PHE:CD2	1:E:239:MSE:HE3	2.21	0.76
1:M:202:MSE:HE3	1:M:203:LEU:C	2.06	0.76
1:C:429:THR:HB	1:C:432:GLN:HG3	1.68	0.76
1:O:179:ILE:HB	1:O:180:PRO:HD3	1.68	0.76
1:P:47:GLN:HE22	1:P:566:VAL:HG13	1.50	0.75
1:G:238:PHE:HD2	1:G:239:MSE:HE2	1.51	0.75
1:C:88:LEU:HD13	1:C:96:PHE:HA	1.69	0.75
1:L:261:ASN:ND2	1:L:261:ASN:H	1.85	0.75
1:A:136:THR:HG22	1:A:138:HIS:H	1.49	0.75
1:K:466:ASN:HA	2:K:1581:NAP:H72N	1.51	0.75
1:M:429:THR:HG22	1:M:431:GLU:H	1.50	0.75
1:O:41:THR:O	1:O:45:ARG:HG3	1.87	0.75
1:E:288:VAL:HG21	1:E:322:LEU:HB3	1.67	0.75
1:F:179:ILE:HB	1:F:180:PRO:HD3	1.68	0.75
1:M:323:ILE:HG22	1:M:327:MSE:HE2	1.68	0.75
1:B:41:THR:HG22	1:B:43:GLU:N	2.01	0.75
1:N:334:LYS:O	1:N:338:ILE:HD12	1.87	0.75
1:F:23:LYS:N	1:F:24:LYS:HZ3	1.85	0.75
1:N:504:GLU:HG3	1:N:508:GLN:NE2	2.01	0.75
1:J:179:ILE:HB	1:J:180:PRO:HD3	1.69	0.74
1:A:238:PHE:CD2	1:A:239:MSE:HE2	2.21	0.74
1:L:550:GLU:O	1:L:554:ARG:HG3	1.88	0.74
1:I:92:ASN:HD22	1:I:92:ASN:C	1.88	0.74
1:I:239:MSE:HE1	1:I:252:ILE:HG21	1.69	0.74
1:F:227:ARG:HH11	1:F:227:ARG:HG3	1.52	0.74
1:O:321:ASN:HB2	7:O:2055:HOH:O	1.84	0.74
1:M:136:THR:HG23	1:M:138:HIS:N	1.99	0.74
1:F:350:ILE:HD11	1:F:362:LYS:HD3	1.69	0.74
1:L:132:GLY:HA3	1:L:177:MSE:CE	2.16	0.74
1:O:324:VAL:HA	1:O:327:MSE:HE3	1.69	0.74
1:A:504:GLU:HG3	1:A:508:GLN:HE21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:ARG:HH11	1:J:270:ARG:HG2	1.52	0.74
1:C:136:THR:CG2	1:C:138:HIS:H	1.96	0.74
1:G:238:PHE:CD2	1:G:239:MSE:HE2	2.22	0.74
1:L:310:GLN:HE22	1:L:393:ALA:HB3	1.52	0.74
1:N:136:THR:HG23	1:N:221:LEU:HD11	1.68	0.74
1:O:266:LEU:O	1:O:270:ARG:HB2	1.88	0.74
1:G:227:ARG:HH11	1:G:227:ARG:HG3	1.53	0.74
1:B:104:ILE:HG13	1:B:108:MSE:HE3	1.70	0.74
1:N:429:THR:HG22	1:N:431:GLU:H	1.53	0.73
1:I:429:THR:HG22	1:I:432:GLN:HG3	1.69	0.73
1:O:412:LYS:HZ3	1:O:412:LYS:HB2	1.51	0.73
1:E:297:ILE:HD11	1:E:507:LEU:HD12	1.69	0.73
1:O:381:VAL:HG13	1:O:407:MSE:HE1	1.69	0.73
7:A:2016:HOH:O	1:D:580:LYS:HG2	1.87	0.73
1:B:136:THR:HG23	1:B:221:LEU:HD11	1.70	0.73
1:O:47:GLN:NE2	1:O:566:VAL:HG13	2.04	0.73
1:A:431:GLU:OE2	1:A:452:VAL:HG22	1.88	0.73
1:D:155:ILE:HD13	1:D:246:TYR:CE2	2.22	0.73
1:A:335:GLU:HG2	1:A:339:LYS:HE3	1.71	0.73
1:L:350:ILE:HG23	1:L:358:LEU:HD11	1.71	0.73
1:M:288:VAL:HG21	1:M:322:LEU:HB3	1.71	0.73
1:E:98:LYS:HD3	1:E:560:THR:CG2	2.18	0.73
1:O:146:MSE:HE3	1:P:51:HIS:CD2	2.23	0.73
1:F:42:LEU:O	1:F:46:GLN:HG3	1.88	0.73
1:P:429:THR:HG22	1:P:431:GLU:H	1.52	0.73
1:F:401:GLN:HG2	1:F:436:TYR:CZ	2.23	0.73
1:M:148:GLN:HG3	1:M:245:ARG:HH21	1.54	0.73
1:M:377:LEU:O	1:M:381:VAL:HG23	1.88	0.73
1:F:183:LYS:HE2	5:F:1586:CL:CL	2.26	0.73
1:O:327:MSE:HB3	1:O:332:VAL:HG11	1.71	0.72
1:O:429:THR:HB	7:O:2063:HOH:O	1.89	0.72
1:A:270:ARG:HH12	1:A:487:GLY:HA2	1.54	0.72
1:N:386:PRO:CG	1:N:407:MSE:HE1	2.18	0.72
1:G:324:VAL:HG12	1:G:328:GLN:NE2	2.04	0.72
1:D:61:GLN:HG2	1:D:98:LYS:HG2	1.69	0.72
1:M:578:LYS:HZ2	1:M:580:LYS:HB2	1.55	0.72
1:G:389:LEU:HD12	1:G:407:MSE:HE3	1.70	0.72
1:N:164:GLU:HG2	1:N:258:ALA:HB2	1.70	0.72
1:M:578:LYS:HZ1	1:M:580:LYS:HD3	1.54	0.72
1:E:429:THR:HG22	1:E:431:GLU:N	2.04	0.72
1:A:386:PRO:CG	1:A:407:MSE:HE1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:GLU:HG2	1:E:258:ALA:HB2	1.71	0.72
1:D:266:LEU:O	1:D:270:ARG:HB2	1.89	0.72
1:D:38:MSE:HB2	1:D:59:LEU:HD11	1.71	0.72
1:G:222:ARG:NH1	1:G:222:ARG:HG3	2.04	0.72
1:D:92:ASN:HD22	1:D:92:ASN:C	1.92	0.72
1:F:98:LYS:HD3	1:F:560:THR:HG21	1.70	0.72
1:L:227:ARG:HG3	1:L:227:ARG:HH11	1.55	0.72
1:A:155:ILE:HD13	1:A:199:LEU:HB2	1.70	0.72
1:N:466:ASN:HA	2:N:1581:NAP:H72N	1.54	0.72
1:B:389:LEU:HD12	1:B:407:MSE:HE3	1.71	0.72
1:J:266:LEU:O	1:J:270:ARG:HB2	1.89	0.72
1:F:61:GLN:O	1:F:65:VAL:HG23	1.90	0.72
1:E:378:GLU:OE2	1:E:402:GLN:HB3	1.88	0.72
1:J:140:ARG:HH11	1:J:140:ARG:HB3	1.55	0.72
1:N:136:THR:CG2	1:N:138:HIS:H	1.95	0.71
1:C:41:THR:HG22	1:C:44:GLU:H	1.55	0.71
1:B:301:ARG:HH11	1:B:301:ARG:HB3	1.54	0.71
1:K:59:LEU:HD13	1:K:64:GLN:HG3	1.70	0.71
1:E:163:GLY:HA2	1:E:166:ILE:HD11	1.70	0.71
1:F:266:LEU:O	1:F:270:ARG:HB2	1.90	0.71
1:A:569:SER:HA	1:C:46:GLN:HE21	1.53	0.71
1:J:238:PHE:HD2	1:J:239:MSE:HE2	1.52	0.71
1:P:41:THR:HG22	1:P:43:GLU:N	2.04	0.71
1:P:454:LEU:HB3	1:P:455:PRO:HD2	1.71	0.71
1:B:239:MSE:HA	1:B:239:MSE:CE	2.20	0.71
1:J:350:ILE:HG23	1:J:358:LEU:HD11	1.73	0.71
1:J:354:ARG:HB3	1:J:358:LEU:HD21	1.71	0.71
1:O:402:GLN:HG3	7:O:2057:HOH:O	1.90	0.71
1:O:327:MSE:O	1:O:332:VAL:HG12	1.89	0.71
1:I:359:THR:HG23	1:I:362:LYS:H	1.56	0.71
1:O:61:GLN:O	1:O:65:VAL:HG23	1.91	0.71
1:A:164:GLU:HG2	1:A:258:ALA:HB2	1.72	0.71
1:L:92:ASN:C	1:L:92:ASN:HD22	1.93	0.71
1:G:177:MSE:CE	1:G:200:PRO:HB2	2.20	0.71
1:D:389:LEU:HD12	1:D:407:MSE:HE3	1.73	0.71
1:N:538:ASN:HB3	7:N:2058:HOH:O	1.88	0.71
1:J:225:ARG:HB2	1:J:227:ARG:HH12	1.55	0.71
1:H:107:PHE:O	1:H:111:VAL:HG23	1.91	0.71
1:P:88:LEU:HD13	1:P:96:PHE:HA	1.72	0.71
1:D:359:THR:HG23	1:D:360:PRO:HD2	1.73	0.70
1:J:41:THR:HG22	1:J:43:GLU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:ARG:HD2	1:H:165:ARG:O	1.91	0.70
1:P:61:GLN:NE2	1:P:98:LYS:HE3	2.05	0.70
1:E:49:ASN:HB3	7:E:2003:HOH:O	1.90	0.70
1:M:238:PHE:CD2	1:M:239:MSE:HE2	2.19	0.70
1:O:177:MSE:HE2	1:O:177:MSE:HA	1.73	0.70
1:B:66:TYR:CE1	1:B:70:LYS:HD3	2.26	0.70
1:H:160:VAL:HG22	1:H:201:VAL:HB	1.73	0.70
1:I:92:ASN:ND2	1:I:95:LEU:H	1.90	0.70
1:B:104:ILE:HG13	1:B:108:MSE:CE	2.20	0.70
1:A:265:LEU:HD22	1:A:269:TYR:HE1	1.55	0.70
1:P:401:GLN:O	1:P:405:GLN:HG3	1.90	0.70
1:P:94:LYS:HD3	1:P:558:TYR:OH	1.91	0.70
1:M:578:LYS:HZ1	1:M:580:LYS:HB2	1.57	0.70
1:M:24:LYS:HZ2	1:O:24:LYS:HD3	1.55	0.70
1:G:359:THR:HG22	1:G:361:GLU:H	1.56	0.70
1:H:136:THR:HG23	1:H:221:LEU:HD11	1.74	0.70
1:G:307:VAL:HG12	1:G:388:VAL:HB	1.73	0.70
1:C:401:GLN:O	1:C:405:GLN:HG3	1.92	0.70
1:A:136:THR:HG22	1:A:138:HIS:N	2.05	0.70
1:J:140:ARG:HB3	1:J:140:ARG:NH1	2.06	0.70
1:C:533:GLU:OE2	1:C:536:ARG:HD2	1.90	0.70
1:F:177:MSE:HA	1:F:177:MSE:CE	2.20	0.69
1:G:160:VAL:HG12	1:G:201:VAL:HB	1.74	0.69
1:A:104:ILE:CG1	1:A:108:MSE:HE3	2.22	0.69
1:I:533:GLU:HA	1:I:536:ARG:NH1	2.06	0.69
1:K:381:VAL:HG11	1:K:407:MSE:HE1	1.75	0.69
1:J:429:THR:HG22	1:J:431:GLU:H	1.58	0.69
1:M:578:LYS:NZ	1:M:580:LYS:HD3	2.07	0.69
1:O:41:THR:HG22	1:O:43:GLU:H	1.58	0.69
1:K:305:HIS:O	1:K:340:ARG:HD2	1.92	0.69
1:M:42:LEU:O	1:M:46:GLN:HG3	1.92	0.69
1:M:578:LYS:NZ	1:M:580:LYS:CB	2.54	0.69
1:H:41:THR:O	1:H:45:ARG:HG3	1.92	0.69
1:L:502:VAL:HG11	1:L:507:LEU:HD13	1.74	0.69
1:O:288:VAL:HG21	1:O:322:LEU:HB3	1.73	0.69
1:A:560:THR:HG22	7:A:2006:HOH:O	1.92	0.69
1:L:401:GLN:HB2	1:L:436:TYR:CD1	2.27	0.69
1:J:133:LEU:HD13	1:J:135:ILE:HD11	1.74	0.69
1:G:35:ASN:ND2	1:G:37:GLY:H	1.91	0.69
1:L:239:MSE:HA	1:L:239:MSE:CE	2.22	0.69
1:F:259:ASN:HD22	1:F:259:ASN:C	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:LYS:HE3	1:K:255:GLU:CD	2.13	0.69
1:I:72:PHE:CZ	1:I:81:ARG:HD3	2.27	0.69
1:I:521:GLN:HG2	7:I:2064:HOH:O	1.93	0.69
1:F:41:THR:HG22	1:F:43:GLU:H	1.58	0.69
1:E:137:ILE:HA	1:E:234:LEU:HD22	1.75	0.69
1:N:98:LYS:HD3	1:N:560:THR:CG2	2.23	0.69
1:H:401:GLN:O	1:H:405:GLN:HG3	1.91	0.69
1:O:385:LYS:HB2	1:O:385:LYS:NZ	2.08	0.69
1:B:466:ASN:HA	2:B:1581:NAP:H72N	1.57	0.69
1:L:483:LEU:HD12	1:L:539:THR:HB	1.74	0.69
1:L:381:VAL:HG11	1:L:407:MSE:HE1	1.73	0.69
1:N:24:LYS:HG2	1:P:24:LYS:HZ2	1.57	0.69
1:F:212:LEU:HD13	1:F:218:TYR:CE1	2.28	0.69
1:M:41:THR:O	1:M:45:ARG:HG3	1.93	0.69
1:B:467:ASN:ND2	3:B:1582:OXL:O2	2.26	0.69
1:N:140:ARG:NH1	1:N:140:ARG:HB3	2.07	0.69
1:D:529:ARG:HA	1:D:532:LYS:HE3	1.73	0.68
1:E:454:LEU:HB3	1:E:455:PRO:HD2	1.74	0.68
1:P:92:ASN:C	1:P:92:ASN:HD22	1.95	0.68
1:M:136:THR:CG2	1:M:138:HIS:H	2.02	0.68
1:M:429:THR:N	1:M:432:GLN:HE21	1.84	0.68
1:P:133:LEU:HD22	1:P:135:ILE:HG13	1.75	0.68
1:G:378:GLU:CA	1:G:403:ILE:HD11	2.24	0.68
1:A:429:THR:HG22	1:A:430:ALA:N	2.07	0.68
1:E:489:ASP:HB3	7:E:2049:HOH:O	1.93	0.68
1:F:129:ARG:NH1	1:F:129:ARG:HG3	2.05	0.68
1:O:88:LEU:HD13	1:O:96:PHE:HA	1.73	0.68
1:G:327:MSE:CE	1:G:337:ALA:HA	2.23	0.68
1:L:38:MSE:SE	1:L:55:PRO:HG2	2.44	0.68
1:J:343:MSE:HB2	1:J:350:ILE:HD12	1.75	0.68
1:L:24:LYS:HG2	1:L:48:LEU:HD12	1.75	0.68
1:C:532:LYS:HD2	1:C:549:LEU:HD12	1.75	0.68
1:O:433:LEU:CD1	1:O:443:PHE:HB2	2.24	0.68
1:G:158:ILE:HD12	1:G:242:VAL:HG11	1.75	0.68
1:G:442:ILE:HG22	1:G:512:LEU:HD11	1.75	0.68
1:L:381:VAL:HG13	1:L:407:MSE:HE1	1.75	0.68
1:P:429:THR:HG22	1:P:431:GLU:N	2.08	0.68
1:A:98:LYS:HD3	1:A:560:THR:CG2	2.23	0.68
1:K:266:LEU:O	1:K:270:ARG:HB2	1.94	0.68
1:C:133:LEU:HD22	1:C:135:ILE:HG13	1.74	0.68
1:G:41:THR:O	1:G:45:ARG:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASP:OD2	1:E:225:ARG:HD2	1.94	0.68
1:M:266:LEU:O	1:M:270:ARG:HB2	1.93	0.68
1:G:266:LEU:O	1:G:270:ARG:HB2	1.93	0.68
1:J:104:ILE:CG1	1:J:108:MSE:HE3	2.22	0.67
1:I:77:SER:O	1:I:81:ARG:HG3	1.93	0.67
1:I:329:LYS:HD3	1:I:492:LEU:HD21	1.75	0.67
1:C:416:ILE:HG13	1:C:433:LEU:CD2	2.21	0.67
1:L:429:THR:HG23	1:L:449:PHE:CE2	2.29	0.67
1:I:466:ASN:HA	2:I:1581:NAP:H72N	1.58	0.67
1:F:453:THR:HG22	1:F:459:THR:OG1	1.94	0.67
1:K:161:THR:HA	1:K:257:PHE:CE1	2.29	0.67
1:G:528:VAL:HG12	1:G:532:LYS:HE2	1.76	0.67
1:B:260:ALA:O	1:B:264:ARG:HG2	1.94	0.67
1:K:381:VAL:CG1	1:K:407:MSE:HE1	2.24	0.67
1:H:154:VAL:O	1:H:154:VAL:HG13	1.94	0.67
1:G:88:LEU:HD13	1:G:96:PHE:HA	1.74	0.67
1:J:556:GLN:HE21	1:J:556:GLN:N	1.92	0.67
1:K:401:GLN:O	1:K:405:GLN:HG3	1.95	0.67
1:A:570:TYR:N	1:C:46:GLN:HE22	1.93	0.67
1:F:336:GLU:HG2	7:F:2050:HOH:O	1.92	0.67
1:N:448:PRO:HD3	1:N:464:GLN:HE22	1.57	0.67
1:N:381:VAL:HG13	1:N:407:MSE:CE	2.19	0.67
1:N:354:ARG:HB3	1:N:358:LEU:HD21	1.75	0.67
1:J:136:THR:HB	1:J:139:ASP:OD2	1.95	0.67
1:A:266:LEU:O	1:A:270:ARG:HB2	1.94	0.67
1:I:502:VAL:HG12	1:I:507:LEU:HD22	1.74	0.67
1:B:433:LEU:HG	1:B:443:PHE:CD1	2.30	0.67
1:G:327:MSE:HE1	1:G:337:ALA:HA	1.76	0.67
1:J:35:ASN:ND2	1:J:37:GLY:H	1.92	0.67
1:G:385:LYS:HA	1:G:410:PHE:CE2	2.29	0.67
1:J:502:VAL:HG12	1:J:507:LEU:HD22	1.76	0.67
1:P:137:ILE:O	1:P:140:ARG:HG2	1.94	0.67
1:G:243:THR:HG22	1:G:248:MSE:HA	1.75	0.67
1:G:202:MSE:HE3	1:G:203:LEU:C	2.15	0.67
1:D:494:THR:HG22	1:D:526:ILE:HG23	1.77	0.67
1:K:165:ARG:O	1:K:165:ARG:HD2	1.95	0.67
1:O:401:GLN:HG2	1:O:405:GLN:NE2	2.07	0.66
1:L:429:THR:H	1:L:432:GLN:HE21	1.43	0.66
1:D:245:ARG:HG2	1:D:246:TYR:CD2	2.30	0.66
1:P:154:VAL:O	1:P:154:VAL:HG13	1.94	0.66
1:M:38:MSE:SE	1:M:55:PRO:HG2	2.46	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:389:LEU:HD12	1:P:407:MSE:HE3	1.78	0.66
1:A:359:THR:HG22	1:A:362:LYS:CE	2.24	0.66
1:C:163:GLY:HA2	1:C:166:ILE:HD11	1.77	0.66
1:K:335:GLU:HG2	1:K:339:LYS:HZ2	1.59	0.66
1:I:239:MSE:HE2	1:I:239:MSE:HA	1.75	0.66
1:H:466:ASN:HA	2:H:1581:NAP:H72N	1.59	0.66
1:L:239:MSE:HE1	1:L:252:ILE:HG12	1.78	0.66
1:J:59:LEU:HD13	1:J:64:GLN:HG2	1.78	0.66
1:G:401:GLN:O	1:G:405:GLN:HG3	1.96	0.66
1:I:578:LYS:NZ	1:L:222:ARG:HD3	2.11	0.66
1:E:469:TYR:OH	1:E:516:LEU:HD13	1.95	0.66
1:L:378:GLU:HA	1:L:403:ILE:CD1	2.25	0.66
1:B:429:THR:HB	1:B:432:GLN:HG2	1.76	0.66
1:I:429:THR:CG2	1:I:432:GLN:HG3	2.25	0.66
1:O:416:ILE:HG13	1:O:433:LEU:HD21	1.78	0.66
1:M:402:GLN:HB3	7:M:2046:HOH:O	1.94	0.66
1:J:184:LEU:HD22	1:J:198:CYS:HB3	1.78	0.66
1:P:300:ASN:OD1	1:P:305:HIS:HE1	1.78	0.66
1:M:177:MSE:O	1:M:180:PRO:HD2	1.96	0.66
1:D:239:MSE:SE	1:D:252:ILE:HD13	2.46	0.66
1:G:179:ILE:HB	1:G:180:PRO:HD3	1.77	0.66
1:M:92:ASN:ND2	1:M:95:LEU:H	1.94	0.66
1:L:41:THR:O	1:L:45:ARG:HG3	1.96	0.66
1:C:266:LEU:O	1:C:270:ARG:HB2	1.95	0.66
1:O:429:THR:HG23	1:O:449:PHE:CE2	2.31	0.66
1:A:288:VAL:HG21	1:A:322:LEU:HB3	1.76	0.66
1:K:415:ILE:HD13	1:K:442:ILE:HD12	1.78	0.66
1:D:47:GLN:NE2	1:D:566:VAL:HG13	2.11	0.66
1:G:391:GLY:HA3	1:G:427:GLU:HG2	1.78	0.66
1:H:391:GLY:HA3	1:H:427:GLU:HG2	1.77	0.66
1:I:222:ARG:HH11	1:L:580:LYS:HE2	1.59	0.66
1:B:24:LYS:NZ	1:D:24:LYS:HD3	2.11	0.66
1:D:332:VAL:HG13	1:D:336:GLU:HB2	1.78	0.66
1:K:154:VAL:HG13	1:K:154:VAL:O	1.95	0.66
1:P:47:GLN:NE2	1:P:566:VAL:HG13	2.10	0.66
1:A:324:VAL:HG12	1:A:328:GLN:HE21	1.61	0.66
1:I:416:ILE:HG13	1:I:433:LEU:HD21	1.78	0.66
1:L:310:GLN:NE2	1:L:393:ALA:HB3	2.10	0.65
1:B:288:VAL:HG21	1:B:322:LEU:HB3	1.79	0.65
1:A:108:MSE:SE	1:A:516:LEU:HD21	2.46	0.65
1:L:454:LEU:HB3	1:L:455:PRO:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:352:LYS:HD2	1:M:366:ALA:O	1.97	0.65
1:D:504:GLU:HG3	1:D:508:GLN:NE2	2.10	0.65
1:P:454:LEU:HD21	1:P:460:LEU:HD11	1.77	0.65
1:B:190:CYS:HB3	1:B:519:ILE:HG12	1.77	0.65
1:O:157:ALA:HB2	1:O:479:ILE:HD11	1.79	0.65
1:D:296:ARG:HB2	1:D:507:LEU:HD21	1.76	0.65
1:L:165:ARG:HD2	1:L:165:ARG:O	1.95	0.65
1:O:166:ILE:HA	1:O:256:ASP:OD2	1.97	0.65
1:J:504:GLU:O	1:J:508:GLN:HG3	1.96	0.65
1:N:270:ARG:HH11	1:N:270:ARG:HG2	1.61	0.65
1:C:137:ILE:HA	1:C:234:LEU:HD22	1.78	0.65
1:B:416:ILE:CG1	1:B:433:LEU:HD21	2.19	0.65
1:D:41:THR:O	1:D:45:ARG:HG3	1.96	0.65
1:L:502:VAL:CG1	1:L:507:LEU:HD13	2.26	0.65
1:J:125:LEU:O	1:J:125:LEU:HD23	1.96	0.65
1:N:179:ILE:HB	1:N:180:PRO:HD3	1.77	0.65
1:I:578:LYS:C	1:I:578:LYS:HD2	2.16	0.65
1:D:546:PRO:HB2	1:D:549:LEU:HD23	1.79	0.65
1:F:327:MSE:HE3	1:F:337:ALA:HB1	1.79	0.65
1:K:319:ILE:O	1:K:323:ILE:HG13	1.97	0.65
1:M:474:VAL:O	1:M:478:VAL:HG23	1.97	0.65
1:A:202:MSE:HE3	1:A:203:LEU:C	2.16	0.65
1:J:389:LEU:HD12	1:J:407:MSE:HE3	1.78	0.65
1:N:288:VAL:HG21	1:N:322:LEU:HB3	1.78	0.65
1:L:136:THR:HB	1:L:139:ASP:OD2	1.96	0.65
1:E:391:GLY:HA3	1:E:427:GLU:HG2	1.79	0.65
1:F:92:ASN:C	1:F:92:ASN:HD22	2.00	0.65
1:N:35:ASN:ND2	1:N:37:GLY:H	1.95	0.65
1:I:429:THR:CG2	1:I:432:GLN:H	2.09	0.65
1:E:133:LEU:HD22	1:E:135:ILE:HG13	1.78	0.65
1:J:347:LYS:O	1:J:375:LYS:NZ	2.30	0.65
1:K:456:SER:OG	1:K:458:GLN:HG2	1.97	0.65
1:J:476:LEU:HD21	1:J:553:ILE:HG23	1.77	0.65
1:C:429:THR:HG22	1:C:431:GLU:H	1.60	0.65
1:K:498:ILE:HD11	1:K:526:ILE:HD11	1.79	0.65
1:C:389:LEU:HD13	1:C:399:PHE:CZ	2.31	0.65
1:C:188:THR:HG21	1:C:195:PRO:HG3	1.78	0.65
1:C:572:TRP:HB2	1:C:577:MSE:HG3	1.78	0.64
1:G:467:ASN:ND2	3:G:1582:OXL:O2	2.29	0.64
1:I:243:THR:HG21	1:I:273:TYR:CD2	2.32	0.64
1:P:572:TRP:O	1:P:573:PRO:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:401:GLN:HG2	1:J:436:TYR:CZ	2.32	0.64
1:I:155:ILE:HD12	1:I:246:TYR:CZ	2.31	0.64
1:N:416:ILE:CG1	1:N:433:LEU:HD21	2.26	0.64
1:J:98:LYS:HD3	1:J:560:THR:CG2	2.27	0.64
1:H:158:ILE:HD12	1:H:242:VAL:HG11	1.80	0.64
1:M:72:PHE:CZ	1:M:81:ARG:HD3	2.33	0.64
1:A:184:LEU:HD12	1:A:200:PRO:HB3	1.79	0.64
1:M:24:LYS:HD2	1:O:24:LYS:NZ	2.12	0.64
1:D:572:TRP:HB2	1:D:577:MSE:HG3	1.78	0.64
1:N:166:ILE:HD12	1:N:179:ILE:HG13	1.78	0.64
1:G:548:ASP:OD2	1:G:551:ALA:HB2	1.96	0.64
1:K:416:ILE:CG1	1:K:433:LEU:HD21	2.25	0.64
1:M:104:ILE:CG1	1:M:108:MSE:HE3	2.27	0.64
1:N:573:PRO:O	1:N:577:MSE:HE2	1.97	0.64
1:L:454:LEU:HD21	1:L:460:LEU:HG	1.78	0.64
1:N:265:LEU:HD22	1:N:269:TYR:HE1	1.61	0.64
1:I:133:LEU:CD2	1:I:135:ILE:HG13	2.27	0.64
1:D:98:LYS:HD3	1:D:560:THR:HG21	1.80	0.64
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.80	0.64
1:P:266:LEU:O	1:P:270:ARG:HB2	1.98	0.64
1:O:75:LEU:HD11	1:O:84:LEU:HD22	1.78	0.64
1:L:416:ILE:CG1	1:L:433:LEU:HD21	2.26	0.64
1:H:389:LEU:HB2	1:H:407:MSE:HE2	1.80	0.64
1:K:378:GLU:HA	1:K:403:ILE:CD1	2.27	0.64
1:A:352:LYS:HG2	1:A:366:ALA:O	1.97	0.64
1:M:466:ASN:HA	2:M:1581:NAP:H72N	1.63	0.64
1:A:350:ILE:HD11	1:A:362:LYS:HD2	1.79	0.64
1:G:155:ILE:HD13	1:G:246:TYR:CE2	2.32	0.64
1:E:416:ILE:HG13	1:E:433:LEU:HD21	1.79	0.64
1:A:335:GLU:O	1:A:339:LYS:HG3	1.98	0.64
1:D:98:LYS:HD3	1:D:560:THR:CG2	2.28	0.64
1:J:41:THR:HB	1:J:44:GLU:HG3	1.78	0.64
1:N:266:LEU:O	1:N:270:ARG:HB2	1.97	0.64
1:H:222:ARG:HG3	1:H:222:ARG:HH11	1.61	0.64
1:C:108:MSE:HE2	1:C:186:LEU:HD13	1.80	0.64
1:L:429:THR:HG22	1:L:431:GLU:H	1.62	0.64
1:J:164:GLU:HG2	1:J:258:ALA:HB2	1.80	0.64
1:N:429:THR:HG22	1:N:430:ALA:N	2.12	0.64
1:A:104:ILE:HG13	1:A:108:MSE:HE3	1.80	0.64
1:I:352:LYS:HE2	1:I:366:ALA:O	1.98	0.64
1:A:92:ASN:HD22	1:A:92:ASN:C	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:GLU:O	1:I:339:LYS:HG3	1.98	0.64
1:B:62:ASP:HB2	7:B:2004:HOH:O	1.98	0.64
1:G:416:ILE:CG1	1:G:433:LEU:HD21	2.16	0.63
1:M:186:LEU:HD22	1:M:190:CYS:SG	2.38	0.63
1:M:429:THR:HG22	1:M:431:GLU:N	2.12	0.63
1:B:238:PHE:CD2	1:B:239:MSE:HE3	2.33	0.63
1:K:335:GLU:HG2	1:K:339:LYS:NZ	2.13	0.63
1:G:72:PHE:CZ	1:G:81:ARG:HD3	2.34	0.63
1:P:416:ILE:CG1	1:P:433:LEU:HD21	2.26	0.63
1:O:466:ASN:HA	2:O:1581:NAP:H72N	1.64	0.63
1:G:184:LEU:HD12	1:G:200:PRO:HB3	1.80	0.63
1:D:352:LYS:HD2	1:D:368:GLU:OE2	1.99	0.63
1:B:300:ASN:HD21	1:B:305:HIS:CE1	2.16	0.63
1:H:324:VAL:O	1:H:328:GLN:HG3	1.98	0.63
1:J:433:LEU:C	1:J:433:LEU:HD13	2.19	0.63
1:E:340:ARG:HH11	1:E:340:ARG:CB	2.11	0.63
1:N:350:ILE:HG23	1:N:358:LEU:HD11	1.81	0.63
1:K:385:LYS:HA	1:K:410:PHE:CE2	2.33	0.63
1:N:41:THR:HG22	1:N:43:GLU:N	2.13	0.63
1:G:177:MSE:HE1	1:G:200:PRO:CB	2.22	0.63
1:L:177:MSE:O	1:L:181:VAL:HG23	1.98	0.63
1:K:36:LYS:HG3	1:K:562:TYR:CD2	2.34	0.63
1:O:385:LYS:HG3	1:O:410:PHE:CG	2.33	0.63
1:A:283:THR:HG23	1:A:284:ALA:N	2.13	0.63
1:G:288:VAL:HG21	1:G:322:LEU:HD12	1.80	0.63
1:H:38:MSE:SE	1:H:55:PRO:HG2	2.49	0.63
1:A:41:THR:HG22	1:A:43:GLU:H	1.64	0.63
1:O:177:MSE:HE3	1:O:202:MSE:HB2	1.79	0.63
1:F:224:LYS:HG2	7:F:2038:HOH:O	1.99	0.63
1:H:474:VAL:O	1:H:478:VAL:HG23	1.99	0.63
1:J:183:LYS:HE3	1:J:255:GLU:CD	2.19	0.63
1:C:92:ASN:HD22	1:C:92:ASN:C	2.01	0.63
1:A:407:MSE:HG2	1:A:416:ILE:HD11	1.80	0.63
1:O:104:ILE:CG1	1:O:108:MSE:HE3	2.21	0.63
1:H:79:LEU:HD21	1:H:125:LEU:HD12	1.80	0.63
1:J:461:TYR:CD1	1:J:509:GLU:HG2	2.34	0.63
1:H:183:LYS:HE2	1:H:255:GLU:OE1	1.99	0.63
1:D:333:SER:OG	1:D:336:GLU:HG3	1.99	0.63
1:M:24:LYS:NZ	1:O:24:LYS:HD3	2.13	0.63
1:O:270:ARG:HG2	1:O:270:ARG:HH11	1.64	0.63
1:N:378:GLU:OE2	1:N:402:GLN:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:O	1:A:380:ILE:HG13	1.98	0.63
1:M:578:LYS:HZ2	1:M:580:LYS:CB	2.12	0.62
1:H:143:ILE:HD12	1:H:237:GLU:HG2	1.80	0.62
1:O:104:ILE:HG13	1:O:108:MSE:CE	2.25	0.62
1:F:389:LEU:HD12	1:F:407:MSE:HE3	1.80	0.62
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.64	0.62
1:M:276:PHE:HB3	1:M:486:ILE:HD12	1.80	0.62
1:B:140:ARG:HH12	1:B:230:ALA:CB	2.09	0.62
1:K:238:PHE:CE2	1:K:239:MSE:HE3	2.34	0.62
1:F:456:SER:OG	1:F:458:GLN:HG2	1.99	0.62
1:M:578:LYS:HZ2	1:M:580:LYS:CA	2.12	0.62
1:P:300:ASN:OD1	1:P:305:HIS:CE1	2.52	0.62
1:O:38:MSE:SE	1:O:55:PRO:HG2	2.50	0.62
1:O:492:LEU:O	1:O:496:GLU:HG3	1.99	0.62
1:D:224:LYS:HE3	7:D:2018:HOH:O	1.99	0.62
1:D:24:LYS:HG2	1:D:48:LEU:HA	1.81	0.62
1:I:41:THR:HG22	1:I:43:GLU:N	2.15	0.62
1:N:324:VAL:O	1:N:328:GLN:HG3	2.00	0.62
1:O:359:THR:HG23	1:O:362:LYS:H	1.64	0.62
1:E:154:VAL:HG13	1:E:154:VAL:O	1.98	0.62
1:B:352:LYS:HE2	1:B:353:GLY:N	2.13	0.62
1:L:524:LEU:HD21	1:L:554:ARG:NE	2.14	0.62
1:K:245:ARG:HG2	1:K:245:ARG:HH11	1.64	0.62
1:E:374:MSE:HE1	1:E:379:ASP:HB3	1.82	0.62
1:I:164:GLU:HG3	1:I:225:ARG:CZ	2.30	0.62
1:M:202:MSE:HE3	1:M:203:LEU:O	1.99	0.62
1:I:104:ILE:CG1	1:I:108:MSE:HE3	2.28	0.62
1:F:494:THR:HG23	1:F:526:ILE:HG23	1.81	0.62
1:A:350:ILE:HG23	1:A:358:LEU:HD11	1.82	0.62
1:J:38:MSE:SE	1:J:55:PRO:HG2	2.50	0.62
1:E:429:THR:HG22	1:E:430:ALA:N	2.14	0.62
1:I:108:MSE:HE2	1:I:190:CYS:SG	2.40	0.62
1:C:469:TYR:OH	1:C:516:LEU:HD13	2.00	0.62
1:C:504:GLU:HG3	1:C:508:GLN:HE21	1.64	0.62
1:J:148:GLN:HG2	1:J:245:ARG:NH2	2.15	0.62
1:H:138:HIS:NE2	1:H:223:HIS:HE1	1.97	0.62
1:A:137:ILE:HB	1:A:205:VAL:HG12	1.82	0.62
1:C:194:LYS:HD2	1:C:197:GLN:HE22	1.64	0.62
1:L:469:TYR:OH	1:L:516:LEU:HD12	2.00	0.62
1:M:416:ILE:CB	1:M:433:LEU:HD21	2.29	0.61
1:L:177:MSE:HG2	1:L:202:MSE:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:MSE:HE1	1:J:252:ILE:HG21	1.82	0.61
1:O:429:THR:H	1:O:432:GLN:CG	2.13	0.61
1:N:467:ASN:ND2	3:N:1582:OXL:O2	2.33	0.61
1:A:401:GLN:O	1:A:405:GLN:HG3	2.00	0.61
1:M:243:THR:HG21	1:M:273:TYR:CD2	2.34	0.61
1:O:296:ARG:HB2	1:O:507:LEU:HD21	1.82	0.61
1:I:41:THR:HG22	1:I:43:GLU:H	1.63	0.61
1:J:152:GLU:OE2	1:J:154:VAL:HG12	2.00	0.61
1:K:321:ASN:HB2	7:K:2024:HOH:O	2.01	0.61
1:B:38:MSE:SE	1:B:55:PRO:HG2	2.50	0.61
1:D:104:ILE:HD11	1:D:108:MSE:HE3	1.82	0.61
1:M:454:LEU:HD12	1:M:454:LEU:H	1.65	0.61
1:D:41:THR:HB	1:D:44:GLU:HG3	1.81	0.61
1:N:324:VAL:HG12	1:N:328:GLN:NE2	2.16	0.61
1:M:98:LYS:HD3	1:M:560:THR:CG2	2.31	0.61
1:M:157:ALA:HB2	1:M:479:ILE:HD11	1.81	0.61
1:G:429:THR:HG22	1:G:430:ALA:N	2.15	0.61
1:H:77:SER:C	1:H:81:ARG:NH1	2.54	0.61
1:B:296:ARG:HB2	1:B:507:LEU:HD21	1.83	0.61
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.82	0.61
1:K:399:PHE:HB2	1:K:428:CYS:HB3	1.82	0.61
1:I:136:THR:HG23	1:I:221:LEU:HD11	1.81	0.61
1:A:429:THR:HB	1:A:432:GLN:HG3	1.83	0.61
1:J:297:ILE:HD11	1:J:507:LEU:HD12	1.82	0.61
1:H:359:THR:HG23	1:H:361:GLU:H	1.64	0.61
1:A:570:TYR:OH	1:D:139:ASP:HB3	2.00	0.61
1:L:238:PHE:CD2	1:L:239:MSE:HE3	2.36	0.61
1:B:42:LEU:O	1:B:46:GLN:HG3	2.01	0.61
1:D:528:VAL:HG12	1:D:532:LYS:HE2	1.82	0.61
1:N:166:ILE:HG21	1:N:172:LEU:HD12	1.83	0.61
1:O:359:THR:HG22	1:O:362:LYS:HE2	1.81	0.61
1:D:108:MSE:HE2	1:D:186:LEU:HD22	1.82	0.61
1:K:27:GLU:OE1	1:K:27:GLU:HA	2.00	0.61
1:F:264:ARG:HH11	1:F:264:ARG:HG2	1.66	0.61
1:K:411:ASN:HB2	1:K:414:PRO:HG3	1.81	0.61
1:J:118:LEU:HD13	1:J:122:HIS:HD2	1.65	0.61
1:G:352:LYS:HA	1:G:352:LYS:HE3	1.83	0.61
1:I:297:ILE:HD11	1:I:507:LEU:HD12	1.83	0.61
1:C:288:VAL:HG21	1:C:322:LEU:HB3	1.81	0.61
1:B:415:ILE:HG12	1:B:442:ILE:HD12	1.83	0.61
1:K:91:ARG:HB2	1:L:129:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:ILE:HA	1:H:234:LEU:HD22	1.82	0.61
1:G:166:ILE:HD12	1:G:179:ILE:HG13	1.83	0.60
1:M:113:THR:HG21	1:M:447:SER:OG	2.01	0.60
1:E:533:GLU:OE1	1:E:536:ARG:NH1	2.34	0.60
1:M:315:ALA:O	1:M:319:ILE:HG13	2.01	0.60
1:C:38:MSE:HE2	1:D:127:PHE:CE2	2.36	0.60
1:C:578:LYS:HB3	1:C:578:LYS:NZ	2.16	0.60
1:L:64:GLN:O	1:L:68:ILE:HG12	2.01	0.60
1:A:177:MSE:HE3	1:A:181:VAL:HG23	1.82	0.60
1:A:416:ILE:HG13	1:A:433:LEU:HD21	1.82	0.60
1:A:359:THR:HG23	1:A:362:LYS:H	1.64	0.60
1:O:428:CYS:HA	1:O:432:GLN:HE21	1.66	0.60
1:D:407:MSE:HG2	1:D:416:ILE:HD11	1.83	0.60
1:P:202:MSE:HE3	1:P:203:LEU:N	2.16	0.60
1:J:285:SER:HB3	1:J:470:VAL:HG21	1.82	0.60
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.82	0.60
1:L:500:GLN:HE21	1:L:500:GLN:N	2.00	0.60
1:G:404:LEU:HD22	1:G:433:LEU:CD2	2.31	0.60
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.82	0.60
1:D:136:THR:HG22	1:D:139:ASP:CG	2.21	0.60
1:H:92:ASN:ND2	1:H:95:LEU:H	1.99	0.60
1:G:359:THR:HG23	1:G:360:PRO:HD2	1.82	0.60
1:A:72:PHE:CZ	1:A:81:ARG:HD3	2.36	0.60
1:I:493:THR:O	1:I:497:VAL:HG23	2.01	0.60
1:H:429:THR:HG22	1:H:430:ALA:N	2.16	0.60
1:G:38:MSE:HB2	1:G:59:LEU:HD11	1.82	0.60
1:F:299:LYS:HB3	1:F:299:LYS:HZ2	1.67	0.60
1:I:184:LEU:HD12	1:I:200:PRO:HB3	1.83	0.60
1:F:285:SER:HB3	1:F:470:VAL:HG21	1.84	0.60
1:K:327:MSE:HE3	1:K:337:ALA:CB	2.25	0.60
1:E:429:THR:CG2	1:E:430:ALA:N	2.65	0.60
1:N:24:LYS:HG2	1:P:24:LYS:HZ1	1.65	0.60
1:P:41:THR:O	1:P:45:ARG:HG3	2.02	0.60
1:E:502:VAL:HG12	1:E:507:LEU:HD22	1.83	0.60
1:M:378:GLU:OE2	1:M:402:GLN:HB3	2.02	0.60
1:F:524:LEU:O	1:F:528:VAL:HG23	2.02	0.60
1:C:340:ARG:HG2	1:C:340:ARG:HH11	1.66	0.60
1:P:575:GLU:O	1:P:578:LYS:HG2	2.02	0.60
1:B:333:SER:HB3	1:E:536:ARG:NH1	2.17	0.60
1:K:359:THR:HG23	1:K:362:LYS:H	1.67	0.60
1:P:59:LEU:HD13	1:P:64:GLN:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:TYR:HB2	7:I:2005:HOH:O	2.01	0.60
1:E:221:LEU:HD13	1:E:223:HIS:HE1	1.66	0.60
1:P:429:THR:H	1:P:432:GLN:NE2	1.99	0.60
1:A:41:THR:HG22	1:A:42:LEU:N	2.17	0.60
1:M:38:MSE:HB2	1:M:59:LEU:HD11	1.83	0.60
1:I:407:MSE:HG2	1:I:416:ILE:HD11	1.84	0.60
1:G:572:TRP:O	1:G:573:PRO:O	2.19	0.60
1:K:417:PHE:CD1	1:K:444:ALA:HB3	2.36	0.60
1:K:532:LYS:HG2	1:K:549:LEU:HD12	1.84	0.60
1:C:467:ASN:HD21	3:C:1582:OXL:C2	2.14	0.60
1:O:260:ALA:HB3	7:O:2050:HOH:O	2.00	0.60
1:B:41:THR:HG21	7:B:2003:HOH:O	2.00	0.60
1:C:429:THR:HG22	1:C:430:ALA:N	2.16	0.60
1:F:401:GLN:O	1:F:405:GLN:HG3	2.02	0.60
1:I:502:VAL:HG22	1:I:514:PRO:HD3	1.84	0.60
1:M:492:LEU:O	1:M:496:GLU:HG3	2.02	0.60
1:O:493:THR:O	1:O:497:VAL:HG23	2.02	0.60
1:G:376:ASN:O	1:G:380:ILE:HG13	2.02	0.59
1:B:160:VAL:HG22	1:B:201:VAL:HB	1.83	0.59
1:N:416:ILE:HG13	1:N:433:LEU:CD2	2.31	0.59
1:C:359:THR:HG22	1:C:362:LYS:H	1.67	0.59
1:O:85:LEU:HD12	1:O:110:ILE:HG21	1.84	0.59
1:F:77:SER:O	1:F:81:ARG:HG3	2.02	0.59
1:I:179:ILE:HB	1:I:180:PRO:HD3	1.83	0.59
1:A:327:MSE:HE3	1:A:337:ALA:CB	2.22	0.59
1:E:416:ILE:HG13	1:E:433:LEU:CD2	2.32	0.59
1:M:245:ARG:HD3	1:M:246:TYR:CE2	2.37	0.59
1:J:184:LEU:HD12	1:J:200:PRO:HB3	1.83	0.59
1:C:223:HIS:HD2	1:C:224:LYS:O	1.85	0.59
1:E:179:ILE:HB	1:E:180:PRO:HD3	1.84	0.59
1:H:59:LEU:HD13	1:H:64:GLN:HG3	1.84	0.59
1:L:131:ARG:HD3	1:L:181:VAL:HG13	1.84	0.59
1:F:554:ARG:HG2	1:F:554:ARG:HH11	1.66	0.59
1:P:239:MSE:SE	1:P:252:ILE:HD13	2.53	0.59
1:J:416:ILE:HG13	1:J:433:LEU:CD2	2.30	0.59
1:L:227:ARG:HG3	1:L:227:ARG:NH1	2.15	0.59
1:C:270:ARG:HG2	1:C:270:ARG:HH11	1.67	0.59
1:N:92:ASN:HD22	1:N:92:ASN:C	2.05	0.59
1:F:35:ASN:ND2	1:F:37:GLY:H	1.98	0.59
1:C:94:LYS:HE2	7:C:2003:HOH:O	2.02	0.59
1:C:433:LEU:HG	1:C:443:PHE:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:42:LEU:O	1:O:46:GLN:HG3	2.02	0.59
1:O:385:LYS:HB2	1:O:385:LYS:HZ3	1.66	0.59
1:L:59:LEU:HD13	1:L:64:GLN:HG2	1.83	0.59
1:H:285:SER:HB3	1:H:470:VAL:HG21	1.85	0.59
1:K:261:ASN:HA	1:K:264:ARG:NH1	2.17	0.59
1:C:136:THR:HG23	1:C:221:LEU:HD11	1.84	0.59
1:A:136:THR:HG23	1:A:138:HIS:H	1.67	0.59
1:F:88:LEU:HD13	1:F:96:PHE:HA	1.84	0.59
1:E:160:VAL:HG11	1:E:238:PHE:CE2	2.38	0.59
1:F:98:LYS:HD3	1:F:560:THR:CG2	2.32	0.59
1:G:41:THR:OG1	1:G:44:GLU:HG3	2.03	0.59
1:L:378:GLU:HA	1:L:403:ILE:HD11	1.84	0.59
1:N:41:THR:HG22	1:N:43:GLU:H	1.66	0.59
1:N:38:MSE:SE	1:N:55:PRO:HG2	2.53	0.59
1:F:136:THR:CG2	1:F:221:LEU:HD11	2.32	0.59
1:M:454:LEU:HD11	1:M:460:LEU:CG	2.28	0.59
1:L:533:GLU:HG3	1:L:537:ASN:HD21	1.68	0.59
1:K:156:LYS:HZ2	1:K:197:GLN:NE2	2.01	0.59
1:K:429:THR:HG22	1:K:430:ALA:N	2.18	0.59
1:B:183:LYS:HE3	1:B:255:GLU:CD	2.22	0.59
1:B:158:ILE:HD12	1:B:242:VAL:HG11	1.84	0.59
1:J:137:ILE:O	1:J:140:ARG:HD2	2.02	0.59
1:I:533:GLU:HG3	1:I:537:ASN:ND2	2.18	0.59
1:D:494:THR:CG2	1:D:526:ILE:HG23	2.32	0.59
1:G:38:MSE:SE	1:G:55:PRO:HG2	2.53	0.59
1:C:454:LEU:HD11	1:C:460:LEU:HD11	1.85	0.59
1:B:202:MSE:HE3	1:B:203:LEU:C	2.23	0.59
1:J:288:VAL:HG21	1:J:322:LEU:HB3	1.84	0.59
1:O:164:GLU:HG2	1:O:258:ALA:HB2	1.84	0.59
1:N:138:HIS:NE2	1:N:223:HIS:HE1	2.01	0.59
1:N:327:MSE:HE3	1:N:337:ALA:CB	2.24	0.59
1:E:297:ILE:CD1	1:E:507:LEU:HD12	2.33	0.59
1:C:133:LEU:HD22	1:C:135:ILE:CG1	2.32	0.59
1:O:165:ARG:O	1:O:165:ARG:HD2	2.02	0.59
1:M:502:VAL:CG1	1:M:507:LEU:HD13	2.32	0.59
1:I:332:VAL:HG13	1:I:336:GLU:HB3	1.83	0.59
1:P:284:ALA:HA	1:P:319:ILE:HG12	1.85	0.58
1:C:23:LYS:HG2	1:C:24:LYS:N	2.11	0.58
1:M:578:LYS:C	1:M:578:LYS:HD2	2.23	0.58
1:B:575:GLU:O	1:B:578:LYS:HG3	2.03	0.58
1:K:578:LYS:O	1:K:578:LYS:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:LYS:CE	1:I:27:GLU:HG2	2.33	0.58
1:A:177:MSE:O	1:A:180:PRO:HD2	2.02	0.58
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.85	0.58
1:L:261:ASN:ND2	1:L:261:ASN:N	2.40	0.58
1:G:160:VAL:CG1	1:G:201:VAL:HB	2.31	0.58
1:J:24:LYS:NZ	1:L:24:LYS:HD2	2.17	0.58
1:B:132:GLY:HA2	1:B:200:PRO:HG2	1.86	0.58
1:M:520:GLN:HG3	7:M:2069:HOH:O	2.02	0.58
1:P:38:MSE:SE	1:P:55:PRO:HG2	2.53	0.58
1:A:36:LYS:HG3	1:A:562:TYR:CD2	2.38	0.58
1:K:416:ILE:HG21	1:K:433:LEU:HD23	1.86	0.58
1:L:104:ILE:HG13	1:L:108:MSE:CE	2.31	0.58
1:H:36:LYS:HG3	1:H:562:TYR:CD2	2.39	0.58
1:A:429:THR:HG22	1:A:431:GLU:H	1.68	0.58
1:D:155:ILE:N	1:D:155:ILE:HD12	2.19	0.58
1:C:356:ALA:HA	1:I:226:ILE:HD12	1.84	0.58
1:P:288:VAL:HG21	1:P:322:LEU:HB3	1.85	0.58
1:E:300:ASN:OD1	1:E:305:HIS:HE1	1.84	0.58
1:D:154:VAL:HG13	1:D:154:VAL:O	2.03	0.58
1:M:69:LEU:O	1:M:73:GLU:HG3	2.03	0.58
1:D:183:LYS:HE3	1:D:255:GLU:CD	2.24	0.58
1:I:285:SER:HB3	1:I:470:VAL:HG21	1.86	0.58
1:E:23:LYS:HD2	1:E:27:GLU:HG2	1.84	0.58
1:P:125:LEU:HD23	1:P:125:LEU:O	2.03	0.58
1:A:381:VAL:HG21	1:A:403:ILE:HG23	1.86	0.58
1:E:137:ILE:HB	1:E:205:VAL:HG12	1.85	0.58
1:L:223:HIS:HD2	1:L:224:LYS:O	1.87	0.58
7:M:2025:HOH:O	1:P:580:LYS:HD3	2.04	0.58
1:I:429:THR:HG22	1:I:432:GLN:CD	2.23	0.58
1:O:401:GLN:HG3	1:O:436:TYR:CD1	2.39	0.58
1:M:158:ILE:HD12	1:M:242:VAL:HG11	1.85	0.58
1:N:354:ARG:HD2	1:N:356:ALA:O	2.03	0.58
1:M:107:PHE:O	1:M:111:VAL:HG12	2.03	0.58
1:K:186:LEU:HD22	1:K:190:CYS:SG	2.44	0.58
1:E:532:LYS:HG3	1:E:549:LEU:HD12	1.84	0.58
1:L:123:TYR:HB3	1:L:175:TYR:CD2	2.39	0.58
1:F:192:GLY:HA3	1:F:557:VAL:HG13	1.84	0.58
1:A:386:PRO:HG2	1:A:407:MSE:CE	2.09	0.58
1:H:416:ILE:CG1	1:H:433:LEU:HD21	2.30	0.58
1:K:239:MSE:HA	1:K:239:MSE:CE	2.31	0.58
1:G:202:MSE:HE3	1:G:203:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PHE:HB2	1:B:428:CYS:HB3	1.86	0.58
1:K:324:VAL:O	1:K:328:GLN:HG3	2.03	0.58
1:F:165:ARG:O	1:F:165:ARG:HD2	2.03	0.58
1:N:209:ASN:OD1	1:N:211:THR:HB	2.03	0.58
1:M:88:LEU:HD13	1:M:96:PHE:HA	1.86	0.58
1:B:412:LYS:O	1:B:413:ARG:HD2	2.03	0.58
1:L:183:LYS:NZ	1:L:467:ASN:HD22	2.00	0.58
1:J:202:MSE:CE	1:J:204:ASP:HB2	2.33	0.58
1:L:186:LEU:HD22	1:L:190:CYS:SG	2.44	0.58
1:K:327:MSE:HE1	1:K:337:ALA:O	2.04	0.58
1:K:145:THR:HA	1:K:148:GLN:HE21	1.67	0.58
1:A:467:ASN:ND2	3:A:1583:OXL:O2	2.37	0.58
1:M:359:THR:HG22	1:M:361:GLU:H	1.68	0.58
1:E:401:GLN:O	1:E:405:GLN:HG3	2.04	0.58
1:E:136:THR:HG23	1:E:221:LEU:HD11	1.85	0.58
1:B:98:LYS:CD	1:B:560:THR:HG21	2.29	0.58
1:N:354:ARG:O	1:N:358:LEU:HD23	2.03	0.58
1:A:202:MSE:HE3	1:A:203:LEU:O	2.04	0.58
1:G:59:LEU:H	1:G:59:LEU:HD12	1.69	0.58
1:H:407:MSE:HG2	1:H:416:ILE:HD11	1.85	0.58
1:J:381:VAL:HG21	1:J:403:ILE:HG23	1.86	0.58
1:K:359:THR:HG22	1:K:362:LYS:HD2	1.86	0.58
1:O:571:THR:HG23	1:O:572:TRP:O	2.02	0.58
1:B:315:ALA:O	1:B:319:ILE:HG13	2.04	0.58
1:N:158:ILE:HD12	1:N:242:VAL:HG11	1.86	0.58
1:L:433:LEU:HG	1:L:443:PHE:CD1	2.39	0.58
1:A:314:GLU:HB2	2:A:1581:NAP:O1N	2.04	0.58
1:H:492:LEU:O	1:H:496:GLU:HG3	2.02	0.58
1:K:174:CYS:HA	1:K:202:MSE:HE3	1.86	0.58
1:C:171:ASP:OD2	1:C:225:ARG:HD2	2.04	0.58
1:P:90:ASP:OD1	1:P:131:ARG:NH1	2.36	0.58
1:K:136:THR:HG22	1:K:139:ASP:OD1	2.04	0.57
1:H:416:ILE:HG21	1:H:433:LEU:HD23	1.85	0.57
1:D:38:MSE:SE	1:D:55:PRO:HG2	2.53	0.57
1:E:349:LEU:HB2	1:E:380:ILE:HD13	1.86	0.57
1:E:38:MSE:SE	1:E:55:PRO:HG2	2.54	0.57
1:E:407:MSE:HG2	1:E:416:ILE:HD11	1.85	0.57
1:G:431:GLU:OE2	1:G:452:VAL:HG22	2.04	0.57
1:L:378:GLU:OE2	1:L:402:GLN:HB3	2.04	0.57
1:J:401:GLN:HG2	1:J:436:TYR:CE1	2.39	0.57
1:J:112:TYR:OH	1:J:183:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:139:ASP:HB3	1:O:570:TYR:OH	2.04	0.57
1:D:117:GLY:O	1:D:121:GLN:HG3	2.04	0.57
1:L:284:ALA:HA	1:L:319:ILE:HG12	1.86	0.57
1:P:136:THR:HG23	1:P:221:LEU:HD11	1.85	0.57
1:D:23:LYS:O	1:D:24:LYS:HG3	2.04	0.57
1:J:416:ILE:CG1	1:J:433:LEU:HD21	2.31	0.57
1:J:433:LEU:HG	1:J:443:PHE:CD1	2.39	0.57
1:J:323:ILE:HG22	1:J:327:MSE:HE2	1.85	0.57
1:E:38:MSE:HB2	1:E:59:LEU:HD11	1.86	0.57
1:H:580:LYS:C	1:H:580:LYS:HD3	2.25	0.57
1:I:100:LEU:HD21	1:I:111:VAL:HG21	1.85	0.57
1:O:238:PHE:CE2	1:O:239:MSE:HE3	2.39	0.57
1:H:238:PHE:O	1:H:242:VAL:HG23	2.04	0.57
1:A:186:LEU:HD22	1:A:190:CYS:SG	2.44	0.57
1:L:496:GLU:O	1:L:500:GLN:NE2	2.36	0.57
1:E:245:ARG:HD3	1:E:246:TYR:CE2	2.39	0.57
1:P:223:HIS:HD2	1:P:224:LYS:O	1.87	0.57
1:N:202:MSE:CE	1:N:204:ASP:HB2	2.35	0.57
1:E:24:LYS:NZ	1:E:49:ASN:HD22	1.88	0.57
1:O:428:CYS:CA	1:O:432:GLN:HE21	2.17	0.57
1:G:381:VAL:CG1	1:G:407:MSE:HE1	2.34	0.57
1:C:108:MSE:CE	1:C:190:CYS:SG	2.93	0.57
1:L:324:VAL:O	1:L:328:GLN:HG3	2.04	0.57
1:I:146:MSE:HE3	1:J:51:HIS:CD2	2.39	0.57
1:E:108:MSE:N	1:E:109:PRO:CD	2.67	0.57
1:B:254:PHE:HE2	1:B:265:LEU:HD13	1.69	0.57
1:K:77:SER:HB2	1:K:80:ASP:OD2	2.05	0.57
1:E:136:THR:HB	1:E:139:ASP:OD2	2.05	0.57
1:O:327:MSE:C	1:O:332:VAL:HG12	2.25	0.57
1:G:242:VAL:HG13	1:G:246:TYR:HD1	1.69	0.57
1:B:431:GLU:HG2	7:B:2034:HOH:O	2.05	0.57
1:C:157:ALA:HB2	1:C:479:ILE:HD11	1.86	0.57
1:H:505:GLU:HG3	7:H:2063:HOH:O	2.05	0.57
1:P:77:SER:O	1:P:81:ARG:HG3	2.05	0.57
1:E:136:THR:CG2	1:E:138:HIS:H	1.99	0.57
1:L:160:VAL:HG22	1:L:201:VAL:HB	1.85	0.57
1:L:227:ARG:HG2	7:L:2031:HOH:O	2.04	0.57
1:I:433:LEU:HD13	1:I:433:LEU:C	2.24	0.57
1:B:575:GLU:CG	1:B:576:ALA:N	2.67	0.57
1:A:375:LYS:HD3	1:A:375:LYS:O	2.04	0.57
1:K:38:MSE:SE	1:K:55:PRO:HG2	2.54	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:358:LEU:HD23	1:P:363:GLU:OE1	2.04	0.57
1:N:442:ILE:HG22	1:N:512:LEU:HD11	1.86	0.57
1:F:416:ILE:CG1	1:F:433:LEU:HD21	2.34	0.57
1:G:327:MSE:HE1	1:G:340:ARG:HG3	1.86	0.57
1:B:64:GLN:NE2	1:B:562:TYR:OH	2.33	0.57
1:L:417:PHE:CD1	1:L:444:ALA:HB3	2.40	0.57
1:B:378:GLU:HA	1:B:403:ILE:HD13	1.87	0.57
1:N:413:ARG:HD2	7:N:2047:HOH:O	2.05	0.57
1:P:466:ASN:HA	2:P:1581:NAP:H72N	1.69	0.57
1:G:429:THR:H	1:G:432:GLN:HE21	1.50	0.57
1:I:72:PHE:CE1	1:I:81:ARG:HB3	2.40	0.57
1:B:428:CYS:CA	1:B:432:GLN:HE21	2.18	0.57
1:K:145:THR:HA	1:K:148:GLN:NE2	2.19	0.57
1:G:499:ALA:HA	7:G:2056:HOH:O	2.05	0.57
1:K:529:ARG:HG2	1:K:529:ARG:HH11	1.68	0.57
1:O:210:GLU:HA	1:O:213:LEU:HD12	1.86	0.57
1:J:555:SER:OG	1:J:556:GLN:NE2	2.38	0.57
1:I:578:LYS:HZ1	1:L:222:ARG:HD3	1.69	0.57
1:O:77:SER:O	1:O:81:ARG:HG3	2.05	0.57
1:A:528:VAL:HG12	1:A:532:LYS:HE2	1.86	0.57
1:F:38:MSE:SE	1:F:55:PRO:HG2	2.55	0.57
1:D:322:LEU:HD22	1:D:492:LEU:HD13	1.87	0.57
1:M:309:PHE:HB2	1:M:343:MSE:HG2	1.85	0.57
1:F:433:LEU:CD1	1:F:443:PHE:HB2	2.35	0.56
1:J:359:THR:CG2	1:J:362:LYS:H	2.13	0.56
1:L:454:LEU:HD21	1:L:460:LEU:CD1	2.34	0.56
1:J:377:LEU:O	1:J:381:VAL:HG23	2.04	0.56
1:I:303:SER:HB2	1:I:332:VAL:HG21	1.87	0.56
1:E:183:LYS:HE3	1:E:255:GLU:OE1	2.05	0.56
1:C:90:ASP:OD1	1:C:131:ARG:NH1	2.38	0.56
1:A:177:MSE:HE3	1:A:177:MSE:O	2.06	0.56
1:D:210:GLU:HA	1:D:213:LEU:HD12	1.86	0.56
1:E:243:THR:HG21	1:E:273:TYR:HD2	1.69	0.56
1:A:165:ARG:HD2	1:A:165:ARG:O	2.06	0.56
1:E:307:VAL:HG22	1:E:388:VAL:HB	1.86	0.56
1:A:35:ASN:ND2	1:A:37:GLY:H	2.04	0.56
1:M:24:LYS:HB2	1:M:24:LYS:HZ1	1.67	0.56
1:F:59:LEU:HD13	1:F:64:GLN:HG3	1.87	0.56
1:C:41:THR:HG22	1:C:43:GLU:N	2.20	0.56
1:M:378:GLU:HA	1:M:403:ILE:CD1	2.35	0.56
1:M:378:GLU:HA	1:M:403:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:433:LEU:HG	1:I:443:PHE:CD1	2.40	0.56
1:B:64:GLN:O	1:B:68:ILE:HG12	2.05	0.56
1:K:517:VAL:HG13	7:K:2037:HOH:O	2.04	0.56
1:B:342:TRP:CH2	1:B:367:HIS:HB2	2.40	0.56
1:B:361:GLU:HA	1:B:364:HIS:HD2	1.70	0.56
1:O:92:ASN:C	1:O:92:ASN:HD22	2.08	0.56
1:K:192:GLY:HA3	1:K:557:VAL:HG13	1.87	0.56
1:P:492:LEU:O	1:P:496:GLU:HG3	2.05	0.56
1:D:493:THR:O	1:D:497:VAL:HG23	2.05	0.56
1:L:407:MSE:HG3	1:L:414:PRO:HB3	1.88	0.56
1:G:171:ASP:OD2	1:G:225:ARG:HD2	2.06	0.56
1:C:86:MSE:HE1	1:C:89:GLN:HE22	1.71	0.56
1:B:429:THR:HG22	1:B:431:GLU:H	1.68	0.56
1:J:155:ILE:HD13	1:J:246:TYR:CE2	2.40	0.56
1:H:429:THR:HG22	1:H:431:GLU:H	1.71	0.56
1:F:77:SER:HB3	1:F:80:ASP:OD2	2.05	0.56
1:C:502:VAL:CG1	1:C:507:LEU:HD13	2.35	0.56
1:C:332:VAL:CG1	1:C:336:GLU:HB3	2.35	0.56
1:N:42:LEU:O	1:N:46:GLN:HG3	2.05	0.56
1:L:429:THR:H	1:L:432:GLN:NE2	2.02	0.56
1:F:381:VAL:CG1	1:F:407:MSE:HE1	2.35	0.56
1:I:322:LEU:HD22	1:I:492:LEU:HD13	1.87	0.56
1:L:41:THR:HG22	1:L:42:LEU:N	2.21	0.56
1:I:222:ARG:NH1	1:L:580:LYS:HE2	2.20	0.56
1:H:152:GLU:HB2	1:H:155:ILE:HD11	1.87	0.56
1:O:354:ARG:HE	1:O:358:LEU:HD11	1.71	0.56
1:C:136:THR:CG2	1:C:137:ILE:N	2.69	0.56
1:P:161:THR:HA	1:P:257:PHE:CE1	2.41	0.56
1:F:433:LEU:HD12	1:F:443:PHE:HB2	1.85	0.56
1:N:448:PRO:HD3	1:N:464:GLN:NE2	2.20	0.56
1:I:23:LYS:O	1:I:24:LYS:HG3	2.06	0.56
1:L:154:VAL:HG23	1:L:154:VAL:O	2.06	0.56
1:A:417:PHE:CD1	1:A:444:ALA:HB3	2.40	0.56
1:J:467:ASN:ND2	3:J:1582:OXL:O2	2.39	0.56
1:N:327:MSE:HE1	1:N:337:ALA:O	2.05	0.56
1:L:524:LEU:HD21	1:L:554:ARG:HE	1.69	0.56
1:A:429:THR:CG2	1:A:430:ALA:N	2.69	0.56
1:G:307:VAL:CG2	1:G:341:ILE:HG12	2.36	0.56
1:I:104:ILE:HD11	1:I:108:MSE:HE3	1.86	0.56
1:K:158:ILE:HD12	1:K:242:VAL:HG11	1.88	0.56
1:P:166:ILE:HD12	1:P:179:ILE:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:334:LYS:HE3	1:L:338:ILE:HD11	1.88	0.56
1:F:466:ASN:HA	2:F:1581:NAP:H72N	1.71	0.56
1:D:547:GLU:N	1:D:547:GLU:CD	2.45	0.56
1:G:381:VAL:HG13	1:G:407:MSE:HE1	1.86	0.56
1:C:533:GLU:HG3	1:C:537:ASN:ND2	2.21	0.56
1:D:210:GLU:OE2	1:D:224:LYS:NZ	2.39	0.56
1:I:159:VAL:HG23	1:I:184:LEU:HD21	1.88	0.56
1:D:429:THR:HG22	1:D:430:ALA:N	2.21	0.56
1:D:466:ASN:HA	2:D:1581:NAP:H72N	1.71	0.56
1:K:504:GLU:HG3	1:K:508:GLN:HE21	1.70	0.56
1:K:377:LEU:O	1:K:381:VAL:HG23	2.06	0.56
1:C:270:ARG:HH12	1:C:487:GLY:HA2	1.71	0.56
1:D:177:MSE:O	1:D:180:PRO:HD2	2.06	0.56
1:E:26:TYR:HB2	7:E:2002:HOH:O	2.06	0.56
1:M:374:MSE:HE1	1:M:379:ASP:C	2.26	0.56
1:H:172:LEU:O	1:H:175:TYR:HB2	2.06	0.56
1:I:161:THR:HA	1:I:257:PHE:CE1	2.41	0.56
1:F:104:ILE:HG13	1:F:108:MSE:HE3	1.86	0.56
1:I:265:LEU:HD22	1:I:269:TYR:HE1	1.71	0.56
1:M:41:THR:OG1	1:M:44:GLU:HG3	2.06	0.56
1:C:194:LYS:HD2	1:C:197:GLN:NE2	2.21	0.56
1:G:183:LYS:NZ	1:G:467:ASN:HD22	2.03	0.56
1:K:359:THR:CG2	1:K:362:LYS:HG3	2.35	0.56
1:C:361:GLU:O	1:C:364:HIS:HB2	2.05	0.56
1:N:520:GLN:HB2	5:N:1586:CL:CL	2.43	0.56
1:O:42:LEU:HD21	1:O:46:GLN:NE2	2.22	0.55
1:J:162:ASP:O	1:J:225:ARG:NH2	2.32	0.55
1:N:429:THR:HG22	1:N:431:GLU:N	2.20	0.55
1:M:300:ASN:OD1	1:M:305:HIS:HE1	1.89	0.55
1:A:229:GLN:HA	1:A:229:GLN:NE2	2.21	0.55
1:B:72:PHE:CZ	1:B:81:ARG:HD3	2.40	0.55
1:E:36:LYS:HD2	1:E:562:TYR:CG	2.41	0.55
1:I:317:LEU:HD23	1:I:343:MSE:HE1	1.88	0.55
1:F:492:LEU:O	1:F:496:GLU:HG3	2.07	0.55
1:H:401:GLN:HG3	1:H:436:TYR:CD1	2.41	0.55
1:A:324:VAL:O	1:A:328:GLN:HG3	2.06	0.55
1:C:394:ALA:HB2	2:C:1581:NAP:O3D	2.06	0.55
1:F:186:LEU:HD22	1:F:190:CYS:SG	2.45	0.55
1:P:396:GLY:O	1:P:426:ALA:O	2.23	0.55
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.88	0.55
1:I:222:ARG:HD2	1:L:580:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:243:THR:HG21	1:I:273:TYR:HD2	1.69	0.55
1:E:158:ILE:HD12	1:E:242:VAL:HG11	1.87	0.55
1:L:416:ILE:HG13	1:L:433:LEU:CD2	2.30	0.55
1:D:323:ILE:HG22	1:D:327:MSE:HE2	1.87	0.55
1:E:239:MSE:HE1	1:E:252:ILE:HG21	1.86	0.55
1:F:212:LEU:HD13	1:F:218:TYR:HE1	1.72	0.55
1:B:428:CYS:HA	1:B:432:GLN:HE21	1.71	0.55
1:C:340:ARG:NH1	1:C:340:ARG:HG2	2.21	0.55
1:L:163:GLY:HA2	1:L:166:ILE:HD11	1.87	0.55
1:M:529:ARG:HH11	1:M:529:ARG:HG2	1.71	0.55
1:P:227:ARG:HG3	1:P:227:ARG:HH11	1.72	0.55
1:J:165:ARG:HD2	1:J:165:ARG:O	2.07	0.55
1:N:36:LYS:HG3	1:N:562:TYR:CD2	2.42	0.55
1:O:239:MSE:HE1	1:O:252:ILE:HG12	1.89	0.55
1:L:179:ILE:HB	1:L:180:PRO:HD3	1.88	0.55
1:H:158:ILE:HG22	1:H:160:VAL:HG23	1.88	0.55
1:J:378:GLU:OE2	1:J:402:GLN:HB3	2.06	0.55
1:G:483:LEU:HD23	1:G:486:ILE:HG12	1.88	0.55
1:N:536:ARG:HG3	1:N:536:ARG:HH11	1.72	0.55
1:G:543:TYR:HA	1:G:544:PRO:C	2.26	0.55
1:P:150:TRP:CE2	1:P:199:LEU:HD13	2.41	0.55
1:P:399:PHE:HB2	1:P:428:CYS:HB3	1.88	0.55
1:C:467:ASN:ND2	3:C:1582:OXL:O2	2.40	0.55
1:J:92:ASN:C	1:J:92:ASN:HD22	2.09	0.55
1:N:374:MSE:CE	1:N:379:ASP:HB3	2.37	0.55
1:E:24:LYS:NZ	1:E:49:ASN:ND2	2.47	0.55
1:I:327:MSE:HE1	1:I:337:ALA:O	2.07	0.55
1:O:431:GLU:HB2	7:O:2063:HOH:O	2.05	0.55
1:O:433:LEU:HG	1:O:443:PHE:CD1	2.42	0.55
1:C:86:MSE:HE1	1:C:89:GLN:NE2	2.21	0.55
1:F:41:THR:HG22	1:F:43:GLU:N	2.22	0.55
1:C:312:ALA:HB3	1:C:362:LYS:HE2	1.89	0.55
1:K:29:LEU:HA	1:K:35:ASN:HD22	1.71	0.55
1:O:90:ASP:OD1	1:O:131:ARG:NH1	2.40	0.55
1:J:329:LYS:HE2	1:J:496:GLU:OE2	2.06	0.55
1:D:389:LEU:CD1	1:D:407:MSE:HE3	2.37	0.55
1:I:158:ILE:HD12	1:I:242:VAL:HG11	1.88	0.55
1:A:528:VAL:CG1	1:A:532:LYS:HE2	2.37	0.55
1:O:357:SER:O	1:O:358:LEU:HD12	2.06	0.55
1:F:162:ASP:O	1:F:225:ARG:NH2	2.39	0.55
1:A:24:LYS:O	1:A:24:LYS:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:ARG:HD3	7:L:2032:HOH:O	2.06	0.55
1:B:125:LEU:HD13	1:B:125:LEU:O	2.07	0.55
1:L:418:ALA:O	1:L:445:SER:HA	2.07	0.55
1:A:27:GLU:OE1	1:B:27:GLU:HG3	2.06	0.55
1:P:416:ILE:HG13	1:P:433:LEU:CD2	2.29	0.55
1:L:429:THR:HG22	1:L:430:ALA:N	2.21	0.55
1:I:354:ARG:HB3	1:I:358:LEU:HD21	1.88	0.55
1:D:61:GLN:O	1:D:65:VAL:HG23	2.07	0.55
1:F:402:GLN:CD	1:F:402:GLN:H	2.11	0.55
1:G:475:ALA:O	1:G:479:ILE:HG13	2.07	0.55
1:O:177:MSE:HA	1:O:177:MSE:HE3	1.86	0.54
1:P:41:THR:HG21	7:P:2006:HOH:O	2.05	0.54
1:F:401:GLN:HG2	1:F:436:TYR:CE2	2.41	0.54
1:C:177:MSE:HG2	1:C:202:MSE:HG3	1.89	0.54
1:B:284:ALA:HA	1:B:319:ILE:HG12	1.89	0.54
1:D:322:LEU:HD21	1:D:492:LEU:HB2	1.88	0.54
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.89	0.54
1:L:288:VAL:HG21	1:L:322:LEU:HB3	1.89	0.54
1:B:529:ARG:HG2	1:B:529:ARG:HH11	1.71	0.54
1:C:141:GLY:H	1:C:237:GLU:CD	2.10	0.54
1:D:388:VAL:HG22	1:D:415:ILE:HB	1.89	0.54
1:J:351:VAL:O	1:J:354:ARG:HB2	2.08	0.54
1:B:66:TYR:CZ	1:B:70:LYS:HD3	2.42	0.54
1:B:314:GLU:HB2	2:B:1581:NAP:O1N	2.07	0.54
1:E:183:LYS:HE2	5:E:1586:CL:CL	2.44	0.54
1:B:156:LYS:HD3	1:B:479:ILE:HG23	1.88	0.54
1:K:171:ASP:OD2	1:K:225:ARG:HD2	2.07	0.54
1:J:303:SER:HB2	1:J:332:VAL:HG21	1.89	0.54
1:F:136:THR:CG2	1:F:137:ILE:N	2.71	0.54
1:M:429:THR:HB	1:M:432:GLN:CG	2.23	0.54
1:A:433:LEU:HD12	1:A:443:PHE:HB2	1.90	0.54
1:K:252:ILE:N	1:K:252:ILE:HD12	2.23	0.54
1:D:433:LEU:HD12	1:D:443:PHE:HB2	1.90	0.54
1:G:239:MSE:HE3	1:G:254:PHE:CZ	2.42	0.54
1:F:24:LYS:HD3	1:H:24:LYS:HD2	1.89	0.54
1:M:64:GLN:O	1:M:68:ILE:HG12	2.07	0.54
1:B:575:GLU:HG3	1:B:576:ALA:N	2.23	0.54
1:K:378:GLU:HA	1:K:403:ILE:HD13	1.89	0.54
1:A:104:ILE:HD11	1:A:108:MSE:HE3	1.88	0.54
1:C:502:VAL:HG11	1:C:507:LEU:HD13	1.90	0.54
1:A:118:LEU:HD22	1:A:122:HIS:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:LEU:HD23	1:H:343:MSE:HE1	1.89	0.54
1:C:391:GLY:HA3	1:C:427:GLU:HG2	1.89	0.54
1:M:396:GLY:O	1:M:426:ALA:O	2.24	0.54
1:K:117:GLY:O	1:K:121:GLN:HG3	2.08	0.54
1:F:61:GLN:HA	1:F:64:GLN:HE21	1.73	0.54
1:A:254:PHE:CE2	1:A:265:LEU:HD13	2.43	0.54
1:A:108:MSE:N	1:A:109:PRO:CD	2.70	0.54
1:I:416:ILE:HG13	1:I:433:LEU:CD2	2.37	0.54
1:J:148:GLN:HG2	1:J:245:ARG:HH21	1.72	0.54
1:H:156:LYS:HD3	1:H:479:ILE:HG23	1.90	0.54
1:N:143:ILE:HD12	1:N:237:GLU:HG2	1.90	0.54
1:H:179:ILE:HB	1:H:180:PRO:HD3	1.89	0.54
1:E:51:HIS:CD2	1:F:146:MSE:HE3	2.42	0.54
1:D:433:LEU:HG	1:D:443:PHE:CD1	2.43	0.54
1:C:533:GLU:HA	1:C:536:ARG:NH1	2.23	0.54
1:D:47:GLN:HE22	1:D:566:VAL:HG13	1.73	0.54
1:D:108:MSE:N	1:D:109:PRO:CD	2.71	0.54
1:I:38:MSE:SE	1:I:55:PRO:HG2	2.58	0.54
1:G:343:MSE:O	1:G:349:LEU:HD12	2.08	0.54
1:O:41:THR:HG22	1:O:43:GLU:N	2.23	0.54
1:A:136:THR:HB	1:A:139:ASP:OD2	2.07	0.54
1:J:270:ARG:HH11	1:J:270:ARG:CG	2.19	0.54
1:E:202:MSE:HE3	1:E:203:LEU:N	2.23	0.54
1:A:162:ASP:O	1:A:225:ARG:NH2	2.41	0.54
1:I:108:MSE:HB3	1:I:109:PRO:HD3	1.89	0.54
1:N:251:LEU:HD23	1:N:478:VAL:HG11	1.88	0.54
1:A:92:ASN:ND2	1:A:92:ASN:C	2.62	0.54
1:I:171:ASP:OD2	1:I:225:ARG:HD2	2.07	0.54
1:L:332:VAL:HG22	1:L:336:GLU:HB2	1.89	0.54
1:K:41:THR:OG1	1:K:44:GLU:HG3	2.08	0.54
1:B:90:ASP:OD2	1:B:131:ARG:NH1	2.30	0.54
1:I:505:GLU:HG3	7:I:2059:HOH:O	2.08	0.54
1:I:396:GLY:O	1:I:426:ALA:O	2.26	0.54
1:N:23:LYS:O	1:N:28:VAL:HG22	2.07	0.54
1:N:192:GLY:HA3	1:N:557:VAL:HG13	1.90	0.54
1:I:502:VAL:HG12	1:I:507:LEU:CD2	2.38	0.54
1:F:94:LYS:HE2	1:F:559:SER:O	2.07	0.54
1:L:177:MSE:O	1:L:180:PRO:HD2	2.08	0.53
1:A:98:LYS:CD	1:A:560:THR:HG21	2.35	0.53
1:N:429:THR:CG2	1:N:430:ALA:N	2.70	0.53
1:A:162:ASP:O	1:A:202:MSE:HE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:171:ASP:OD2	1:P:225:ARG:HD2	2.08	0.53
1:P:179:ILE:HB	1:P:180:PRO:HD3	1.90	0.53
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.90	0.53
1:N:77:SER:O	1:N:81:ARG:HG3	2.08	0.53
1:L:352:LYS:NZ	1:L:352:LYS:HB3	2.23	0.53
1:O:136:THR:CG2	1:O:221:LEU:HD11	2.35	0.53
1:O:44:GLU:O	1:O:48:LEU:HD13	2.08	0.53
1:F:239:MSE:CE	1:F:252:ILE:HD13	2.37	0.53
1:L:92:ASN:C	1:L:92:ASN:ND2	2.60	0.53
1:B:77:SER:HB3	1:B:80:ASP:OD2	2.08	0.53
1:J:276:PHE:HB3	1:J:486:ILE:HD12	1.90	0.53
1:J:33:HIS:CD2	1:J:93:GLU:OE1	2.61	0.53
1:M:137:ILE:HA	1:M:234:LEU:HD22	1.90	0.53
1:F:157:ALA:HB2	1:F:479:ILE:HD11	1.89	0.53
1:B:405:GLN:NE2	1:B:436:TYR:O	2.39	0.53
1:C:158:ILE:HD12	1:C:242:VAL:HG11	1.90	0.53
1:C:183:LYS:HE3	1:C:255:GLU:CD	2.29	0.53
1:E:327:MSE:O	1:E:332:VAL:HG12	2.08	0.53
1:B:61:GLN:HE22	1:B:560:THR:CG2	2.21	0.53
1:I:133:LEU:HD23	1:I:134:PHE:N	2.23	0.53
1:J:359:THR:HG22	1:J:362:LYS:CG	2.38	0.53
1:E:502:VAL:HG22	1:E:514:PRO:HD3	1.90	0.53
1:J:24:LYS:HG2	1:J:48:LEU:HA	1.89	0.53
1:G:270:ARG:HH11	1:G:270:ARG:HG2	1.73	0.53
1:C:132:GLY:HA3	1:C:177:MSE:CE	2.37	0.53
1:N:90:ASP:OD1	1:N:131:ARG:NH1	2.28	0.53
1:M:172:LEU:O	1:M:175:TYR:HB2	2.09	0.53
1:N:543:TYR:HA	1:N:544:PRO:C	2.29	0.53
1:L:381:VAL:HG11	1:L:407:MSE:CE	2.39	0.53
1:F:407:MSE:HG2	1:F:416:ILE:HD11	1.90	0.53
1:H:315:ALA:O	1:H:319:ILE:HG13	2.09	0.53
1:C:132:GLY:HA3	1:C:177:MSE:HE1	1.91	0.53
1:O:354:ARG:NE	1:O:358:LEU:HD11	2.23	0.53
1:O:156:LYS:HE2	1:O:197:GLN:NE2	2.24	0.53
1:I:467:ASN:H	2:I:1581:NAP:H72N	1.54	0.53
1:J:64:GLN:NE2	1:J:562:TYR:OH	2.41	0.53
1:B:428:CYS:HB2	1:B:432:GLN:HE21	1.73	0.53
1:J:389:LEU:CD1	1:J:407:MSE:HE3	2.38	0.53
1:O:359:THR:CG2	1:O:362:LYS:HG3	2.38	0.53
1:B:36:LYS:HD3	1:B:562:TYR:HB3	1.89	0.53
1:N:413:ARG:CD	7:N:2047:HOH:O	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ARG:O	1:F:30:ARG:HD2	2.09	0.53
1:H:529:ARG:HH11	1:H:529:ARG:HG2	1.74	0.53
1:C:536:ARG:NE	1:H:333:SER:HB3	2.24	0.53
1:N:85:LEU:HD12	1:N:110:ILE:HG21	1.90	0.53
1:G:184:LEU:HD22	1:G:198:CYS:HB3	1.90	0.53
1:E:24:LYS:CG	1:E:25:GLY:N	2.60	0.53
1:M:454:LEU:CD1	1:M:460:LEU:HG	2.31	0.53
1:F:227:ARG:NH1	1:F:227:ARG:HG3	2.23	0.53
1:J:24:LYS:HZ2	1:L:24:LYS:CD	2.21	0.53
1:J:177:MSE:HE2	1:J:202:MSE:HB2	1.90	0.53
1:G:319:ILE:O	1:G:323:ILE:HG13	2.09	0.53
1:B:302:LEU:O	1:B:327:MSE:HE2	2.09	0.53
1:M:342:TRP:HA	7:M:2041:HOH:O	2.08	0.53
1:C:77:SER:O	1:C:81:ARG:HG3	2.07	0.53
1:C:164:GLU:HG2	1:C:258:ALA:HB2	1.90	0.53
1:O:123:TYR:HB3	1:O:175:TYR:CD2	2.44	0.53
1:D:136:THR:OG1	1:D:221:LEU:HD11	2.08	0.53
1:J:429:THR:HG22	1:J:430:ALA:N	2.23	0.53
1:G:431:GLU:OE2	1:G:452:VAL:HG13	2.09	0.53
1:E:162:ASP:C	1:E:202:MSE:HE1	2.29	0.53
1:L:41:THR:HG22	1:L:43:GLU:H	1.74	0.53
1:C:381:VAL:HG13	1:C:407:MSE:HE1	1.90	0.53
1:J:154:VAL:O	1:J:154:VAL:HG13	2.08	0.53
1:N:492:LEU:O	1:N:496:GLU:HG3	2.09	0.53
1:I:91:ARG:NH2	7:I:2015:HOH:O	2.40	0.53
1:C:245:ARG:HD3	1:C:246:TYR:CE2	2.44	0.53
1:J:543:TYR:HA	1:J:544:PRO:C	2.30	0.53
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.90	0.53
1:O:412:LYS:HB2	1:O:412:LYS:HZ2	1.69	0.53
1:M:24:LYS:HE2	1:O:24:LYS:HZ3	1.73	0.53
1:J:359:THR:HG22	1:J:362:LYS:HB2	1.91	0.53
1:K:467:ASN:H	2:K:1581:NAP:H72N	1.57	0.53
1:J:24:LYS:HD2	1:L:24:LYS:HD2	1.91	0.53
1:B:300:ASN:ND2	1:B:305:HIS:CE1	2.77	0.53
1:A:493:THR:O	1:A:497:VAL:HG23	2.08	0.53
1:E:570:TYR:H	1:G:46:GLN:HE22	1.55	0.53
1:L:156:LYS:HD3	1:L:479:ILE:HG23	1.90	0.53
1:D:160:VAL:HG11	1:D:238:PHE:CE2	2.43	0.53
1:K:402:GLN:H	1:K:402:GLN:NE2	2.06	0.53
1:D:359:THR:HG21	7:D:2029:HOH:O	2.08	0.53
1:I:404:LEU:HD13	1:I:433:LEU:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:554:ARG:HH11	1:I:554:ARG:HG2	1.74	0.53
1:F:429:THR:HG22	1:F:430:ALA:N	2.24	0.52
1:P:401:GLN:HG3	1:P:402:GLN:NE2	2.25	0.52
1:A:104:ILE:CD1	1:A:108:MSE:HE3	2.39	0.52
1:B:38:MSE:HB2	1:B:59:LEU:HD11	1.91	0.52
1:A:521:GLN:O	1:A:525:LYS:HG3	2.09	0.52
1:F:469:TYR:OH	1:F:516:LEU:HD13	2.09	0.52
1:N:252:ILE:HD12	1:N:252:ILE:N	2.24	0.52
1:O:324:VAL:HG12	1:O:328:GLN:HE21	1.73	0.52
1:O:239:MSE:HA	1:O:239:MSE:CE	2.37	0.52
1:A:137:ILE:HA	1:A:234:LEU:HD22	1.92	0.52
1:D:245:ARG:HG2	1:D:246:TYR:CE2	2.44	0.52
1:C:108:MSE:HE1	1:C:190:CYS:SG	2.49	0.52
1:K:429:THR:HG22	1:K:431:GLU:H	1.74	0.52
1:E:243:THR:HG21	1:E:273:TYR:CD2	2.43	0.52
1:O:156:LYS:HE2	1:O:197:GLN:CD	2.30	0.52
1:B:474:VAL:O	1:B:478:VAL:HG23	2.10	0.52
1:E:270:ARG:HH12	1:E:487:GLY:HA2	1.74	0.52
1:A:38:MSE:SE	1:A:55:PRO:HG2	2.59	0.52
1:N:433:LEU:HG	1:N:443:PHE:CD1	2.45	0.52
1:J:284:ALA:HA	1:J:319:ILE:HG12	1.91	0.52
1:B:41:THR:CG2	1:B:43:GLU:H	2.19	0.52
1:P:98:LYS:HD3	1:P:560:THR:HG21	1.90	0.52
1:G:528:VAL:O	1:G:532:LYS:HG3	2.09	0.52
1:J:202:MSE:HE1	1:J:204:ASP:CA	2.39	0.52
1:D:429:THR:HG22	1:D:431:GLU:H	1.73	0.52
1:L:192:GLY:HA3	1:L:557:VAL:HG22	1.92	0.52
1:G:433:LEU:HD12	1:G:443:PHE:HB2	1.92	0.52
1:O:401:GLN:O	1:O:405:GLN:HG3	2.09	0.52
1:C:108:MSE:HE2	1:C:186:LEU:CD1	2.40	0.52
1:N:41:THR:HB	1:N:44:GLU:HG3	1.91	0.52
1:C:504:GLU:HG3	1:C:508:GLN:NE2	2.23	0.52
1:C:288:VAL:HG12	1:C:292:LEU:HD22	1.92	0.52
1:H:329:LYS:NZ	1:H:496:GLU:OE2	2.40	0.52
1:L:82:TYR:CE2	1:L:86:MSE:HG3	2.44	0.52
1:I:29:LEU:HD23	1:I:35:ASN:HD22	1.73	0.52
1:N:154:VAL:O	1:N:154:VAL:HG13	2.10	0.52
1:A:88:LEU:HD13	1:A:96:PHE:HA	1.90	0.52
1:G:223:HIS:HD2	1:G:224:LYS:O	1.92	0.52
1:N:343:MSE:O	1:N:349:LEU:HD12	2.10	0.52
1:G:61:GLN:HE22	1:G:98:LYS:HD3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:332:VAL:HG22	1:P:336:GLU:HB3	1.91	0.52
1:J:429:THR:H	1:J:432:GLN:CG	2.23	0.52
1:J:120:CYS:O	1:J:175:TYR:HB3	2.09	0.52
1:N:352:LYS:O	1:N:352:LYS:HG2	2.07	0.52
1:M:556:GLN:CA	1:M:556:GLN:HE21	2.22	0.52
1:N:160:VAL:HG21	1:N:238:PHE:CE2	2.44	0.52
1:J:86:MSE:HE1	1:J:131:ARG:HH11	1.75	0.52
1:E:528:VAL:HG22	1:E:553:ILE:HD12	1.90	0.52
1:L:327:MSE:HE3	1:L:337:ALA:CB	2.27	0.52
1:F:166:ILE:HG21	1:F:172:LEU:HD12	1.91	0.52
1:O:238:PHE:HD2	1:O:239:MSE:HE3	1.73	0.52
1:F:125:LEU:HD13	1:F:125:LEU:O	2.09	0.52
1:O:207:THR:HA	1:O:225:ARG:HG2	1.92	0.52
1:E:209:ASN:OD1	1:E:211:THR:HB	2.09	0.52
1:L:398:ALA:HB3	1:L:427:GLU:HG3	1.90	0.52
1:A:433:LEU:HD12	1:A:434:TYR:CD2	2.44	0.52
1:B:108:MSE:N	1:B:109:PRO:CD	2.73	0.52
1:D:108:MSE:CE	1:D:190:CYS:SG	2.97	0.52
1:H:529:ARG:HG2	1:H:529:ARG:NH1	2.25	0.52
1:F:319:ILE:O	1:F:323:ILE:HG13	2.10	0.52
1:H:161:THR:HA	1:H:257:PHE:CE1	2.45	0.52
1:B:312:ALA:HB2	1:B:343:MSE:HG2	1.91	0.52
1:P:158:ILE:HG23	1:P:199:LEU:O	2.10	0.52
1:O:428:CYS:HA	1:O:432:GLN:NE2	2.25	0.52
1:G:270:ARG:HH12	1:G:487:GLY:HA2	1.73	0.52
1:M:243:THR:HG21	1:M:273:TYR:HD2	1.75	0.52
1:E:324:VAL:O	1:E:328:GLN:HG3	2.10	0.52
1:E:492:LEU:O	1:E:496:GLU:HG3	2.09	0.52
1:K:330:GLU:O	1:O:300:ASN:HA	2.10	0.52
1:I:238:PHE:CE2	1:I:239:MSE:HE3	2.45	0.52
1:O:166:ILE:HD12	1:O:179:ILE:HG13	1.91	0.52
1:J:41:THR:HG22	1:J:43:GLU:N	2.24	0.52
1:I:536:ARG:HD2	7:I:2069:HOH:O	2.09	0.52
1:G:288:VAL:CG2	1:G:322:LEU:HD12	2.40	0.52
1:H:141:GLY:H	1:H:237:GLU:CD	2.13	0.52
1:B:332:VAL:CG1	1:B:336:GLU:HB3	2.40	0.52
1:N:72:PHE:CE2	1:N:81:ARG:HD3	2.45	0.52
1:N:352:LYS:O	1:N:352:LYS:CG	2.58	0.52
1:G:394:ALA:HB2	2:G:1581:NAP:O3D	2.10	0.52
1:H:571:THR:HG23	7:H:2075:HOH:O	2.09	0.52
1:K:136:THR:HG22	1:K:139:ASP:CG	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:HIS:NE2	1:M:223:HIS:HE1	2.08	0.52
1:I:284:ALA:HA	1:I:319:ILE:HG12	1.91	0.52
1:O:407:MSE:HG2	1:O:416:ILE:HD11	1.91	0.52
1:J:317:LEU:HD23	1:J:343:MSE:HE1	1.92	0.52
1:A:284:ALA:HA	1:A:319:ILE:HG12	1.92	0.52
1:B:59:LEU:H	1:B:59:LEU:HD12	1.74	0.52
1:I:38:MSE:HB2	1:I:59:LEU:HD11	1.92	0.52
1:M:35:ASN:ND2	1:M:37:GLY:H	2.07	0.52
1:O:41:THR:HG22	1:O:42:LEU:N	2.25	0.51
1:O:429:THR:HG22	1:O:430:ALA:N	2.25	0.51
1:I:467:ASN:N	2:I:1581:NAP:H72N	2.09	0.51
1:I:222:ARG:HD2	1:L:580:LYS:HE2	1.92	0.51
1:M:468:SER:HA	1:M:471:PHE:CE2	2.45	0.51
1:J:245:ARG:HG2	1:J:246:TYR:CD2	2.45	0.51
1:H:429:THR:H	1:H:432:GLN:NE2	2.07	0.51
1:C:35:ASN:ND2	1:C:37:GLY:H	2.08	0.51
1:I:320:ALA:O	1:I:324:VAL:HG23	2.10	0.51
1:N:112:TYR:CE2	1:N:468:SER:OG	2.63	0.51
1:P:155:ILE:HB	1:P:246:TYR:CD2	2.46	0.51
1:A:416:ILE:HG13	1:A:433:LEU:CD2	2.39	0.51
1:K:381:VAL:HG11	1:K:407:MSE:CE	2.41	0.51
1:B:352:LYS:CE	1:B:353:GLY:H	2.20	0.51
1:J:461:TYR:HD1	1:J:509:GLU:HG2	1.75	0.51
1:H:529:ARG:HD3	7:H:2068:HOH:O	2.09	0.51
1:F:75:LEU:HD11	1:F:84:LEU:HD22	1.92	0.51
1:G:92:ASN:C	1:G:92:ASN:HD22	2.12	0.51
1:I:377:LEU:O	1:I:381:VAL:HG23	2.11	0.51
1:N:162:ASP:O	1:N:225:ARG:NH2	2.33	0.51
1:B:145:THR:O	1:B:148:GLN:HG2	2.10	0.51
1:C:152:GLU:HB3	1:C:155:ILE:CD1	2.40	0.51
1:O:158:ILE:HG22	1:O:160:VAL:HG23	1.91	0.51
1:F:431:GLU:OE2	1:F:452:VAL:HG22	2.10	0.51
1:F:416:ILE:HG13	1:F:433:LEU:CD2	2.36	0.51
1:H:284:ALA:HA	1:H:319:ILE:HG12	1.92	0.51
1:O:65:VAL:HG13	1:O:99:VAL:HG22	1.91	0.51
1:J:556:GLN:NE2	1:J:556:GLN:N	2.57	0.51
1:B:429:THR:H	1:B:432:GLN:CG	2.23	0.51
1:J:96:PHE:CZ	1:J:100:LEU:HD11	2.44	0.51
1:M:429:THR:HG22	1:M:430:ALA:N	2.25	0.51
1:L:136:THR:CG2	1:L:137:ILE:N	2.73	0.51
1:F:381:VAL:HG13	1:F:407:MSE:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:GLN:NE2	1:C:436:TYR:CE1	2.78	0.51
1:C:533:GLU:HA	1:C:536:ARG:HH11	1.74	0.51
1:M:98:LYS:HD3	1:M:560:THR:HG23	1.91	0.51
1:J:303:SER:CB	1:J:332:VAL:HG21	2.41	0.51
1:K:454:LEU:HB3	1:K:455:PRO:HD2	1.90	0.51
1:N:215:ASP:O	1:N:222:ARG:NH2	2.43	0.51
1:I:300:ASN:OD1	1:I:305:HIS:HE1	1.92	0.51
1:C:251:LEU:C	1:C:252:ILE:HD12	2.31	0.51
1:G:433:LEU:O	1:G:437:THR:HG23	2.10	0.51
1:K:136:THR:OG1	1:K:221:LEU:HD11	2.10	0.51
1:H:361:GLU:O	1:H:364:HIS:HB2	2.11	0.51
1:O:42:LEU:C	1:O:42:LEU:HD23	2.30	0.51
1:I:288:VAL:HG21	1:I:322:LEU:HB3	1.93	0.51
1:M:179:ILE:HB	1:M:180:PRO:HD3	1.92	0.51
1:C:543:TYR:HA	1:C:544:PRO:C	2.31	0.51
1:M:125:LEU:N	5:M:1591:CL:CL	2.81	0.51
1:J:388:VAL:HG22	1:J:415:ILE:HB	1.93	0.51
1:B:354:ARG:HD2	1:B:356:ALA:O	2.10	0.51
1:G:136:THR:HB	1:G:139:ASP:OD2	2.10	0.51
1:M:454:LEU:HB3	1:M:455:PRO:HD2	1.93	0.51
1:A:350:ILE:CD1	1:A:362:LYS:HD2	2.41	0.51
1:B:238:PHE:O	1:B:242:VAL:HG23	2.11	0.51
1:L:174:CYS:HA	1:L:202:MSE:HE3	1.91	0.51
1:E:133:LEU:HB2	1:E:199:LEU:HD11	1.92	0.51
1:C:431:GLU:HG3	7:C:2052:HOH:O	2.11	0.51
1:I:92:ASN:C	1:I:92:ASN:ND2	2.62	0.51
1:F:401:GLN:HG2	1:F:436:TYR:CE1	2.45	0.51
1:L:140:ARG:NH2	1:L:230:ALA:HA	2.25	0.51
1:E:92:ASN:C	1:E:92:ASN:HD22	2.13	0.51
1:E:44:GLU:O	1:E:48:LEU:HB2	2.11	0.51
1:J:529:ARG:HG2	1:J:529:ARG:HH11	1.76	0.51
1:D:141:GLY:H	1:D:237:GLU:CD	2.13	0.51
1:D:150:TRP:CE2	1:D:199:LEU:HD13	2.46	0.51
1:L:301:ARG:HB3	1:L:330:GLU:OE1	2.11	0.51
1:N:136:THR:CG2	1:N:221:LEU:HD11	2.36	0.51
1:D:319:ILE:O	1:D:323:ILE:HG13	2.10	0.51
1:E:160:VAL:HG12	1:E:201:VAL:CB	2.39	0.51
1:N:140:ARG:HH11	1:N:140:ARG:HB3	1.74	0.51
1:F:223:HIS:HD2	1:F:224:LYS:O	1.93	0.51
1:L:190:CYS:HB3	1:L:519:ILE:HD13	1.93	0.51
1:F:322:LEU:HD11	1:F:492:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:THR:HG22	1:B:114:PRO:HA	1.92	0.51
1:D:171:ASP:OD2	1:D:225:ARG:HD2	2.11	0.51
1:N:88:LEU:HD22	1:N:96:PHE:HB2	1.93	0.51
1:P:160:VAL:HG12	1:P:161:THR:N	2.26	0.51
1:D:92:ASN:ND2	1:D:95:LEU:H	2.08	0.51
1:I:536:ARG:CD	7:I:2069:HOH:O	2.58	0.51
1:B:429:THR:HG22	1:B:430:ALA:N	2.26	0.51
1:A:319:ILE:O	1:A:323:ILE:HG13	2.11	0.51
1:H:78:ASP:N	1:H:81:ARG:NH1	2.58	0.51
1:L:166:ILE:HG21	1:L:172:LEU:HD12	1.93	0.51
1:E:399:PHE:HB2	1:E:428:CYS:HB3	1.93	0.51
1:D:554:ARG:HH11	1:D:554:ARG:HG2	1.76	0.51
1:B:117:GLY:O	1:B:121:GLN:HG3	2.11	0.51
1:F:166:ILE:HD12	1:F:179:ILE:CG1	2.40	0.51
1:P:36:LYS:HE2	1:P:562:TYR:HB3	1.93	0.51
1:F:429:THR:H	1:F:432:GLN:HE21	1.56	0.51
1:G:42:LEU:O	1:G:46:GLN:HG3	2.10	0.51
1:E:270:ARG:NH2	1:E:281:GLN:NE2	2.59	0.51
1:P:476:LEU:HB3	1:P:527:ALA:HB2	1.93	0.51
1:I:36:LYS:HD2	1:I:562:TYR:CG	2.46	0.51
1:H:214:LYS:NZ	1:H:214:LYS:HB2	2.26	0.51
1:E:132:GLY:HA2	1:E:200:PRO:HG2	1.93	0.51
1:H:270:ARG:HH12	1:H:487:GLY:HA2	1.76	0.51
1:I:136:THR:HB	1:I:139:ASP:OD2	2.11	0.51
1:N:59:LEU:C	1:N:59:LEU:HD12	2.32	0.51
1:J:502:VAL:HG12	1:J:507:LEU:CD2	2.39	0.51
1:L:454:LEU:HD21	1:L:460:LEU:CG	2.41	0.51
1:A:207:THR:HA	1:A:225:ARG:HH11	1.76	0.51
1:D:166:ILE:HD12	1:D:179:ILE:HG13	1.93	0.51
1:D:431:GLU:OE2	1:D:452:VAL:HG13	2.10	0.51
1:K:41:THR:O	1:K:45:ARG:HG3	2.11	0.51
1:G:314:GLU:HB2	2:G:1581:NAP:O1N	2.10	0.51
1:N:401:GLN:HG2	1:N:436:TYR:CE2	2.46	0.51
1:A:391:GLY:HA3	1:A:427:GLU:HG2	1.92	0.51
1:G:476:LEU:HB3	1:G:527:ALA:HB2	1.93	0.51
1:A:31:ASP:HA	1:B:30:ARG:NH1	2.26	0.51
1:E:404:LEU:HD13	1:E:433:LEU:HA	1.93	0.50
1:C:433:LEU:HG	1:C:443:PHE:HD1	1.76	0.50
1:H:140:ARG:NH1	1:H:230:ALA:HA	2.26	0.50
1:K:342:TRP:CH2	1:K:367:HIS:HB2	2.46	0.50
1:A:416:ILE:CG1	1:A:433:LEU:HD21	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:327:MSE:HE1	1:P:337:ALA:O	2.11	0.50
1:F:238:PHE:CE2	1:F:239:MSE:HE3	2.45	0.50
1:J:270:ARG:HG2	1:J:270:ARG:NH1	2.25	0.50
1:J:378:GLU:HA	1:J:403:ILE:HD13	1.92	0.50
1:N:288:VAL:O	1:N:292:LEU:HD13	2.12	0.50
1:A:401:GLN:HG2	1:A:436:TYR:CE1	2.46	0.50
1:P:162:ASP:C	1:P:202:MSE:HE1	2.31	0.50
1:C:467:ASN:H	2:C:1581:NAP:H72N	1.59	0.50
1:F:553:ILE:O	1:F:557:VAL:HG23	2.11	0.50
1:I:543:TYR:HA	1:I:544:PRO:C	2.32	0.50
1:C:556:GLN:HE21	1:C:556:GLN:N	2.09	0.50
1:N:210:GLU:OE2	1:N:224:LYS:HE2	2.12	0.50
1:N:86:MSE:HE2	7:N:2024:HOH:O	2.11	0.50
1:C:61:GLN:NE2	1:C:98:LYS:HD2	2.27	0.50
1:I:270:ARG:NH1	5:I:1588:CL:CL	2.81	0.50
1:F:166:ILE:HD12	1:F:179:ILE:HG13	1.93	0.50
1:O:429:THR:H	1:O:432:GLN:NE2	2.10	0.50
1:C:41:THR:HB	1:C:44:GLU:HG3	1.92	0.50
1:A:108:MSE:HE2	1:A:190:CYS:SG	2.51	0.50
1:A:283:THR:CG2	1:A:284:ALA:N	2.74	0.50
1:I:389:LEU:HD12	1:I:407:MSE:HE3	1.93	0.50
1:I:104:ILE:HG13	1:I:108:MSE:HE3	1.93	0.50
1:K:264:ARG:HH11	1:K:264:ARG:HG2	1.76	0.50
1:D:314:GLU:HB2	2:D:1581:NAP:O1N	2.11	0.50
1:M:140:ARG:HG3	1:M:234:LEU:HD13	1.92	0.50
1:A:90:ASP:OD1	1:A:131:ARG:NH1	2.44	0.50
1:D:378:GLU:OE1	1:D:382:LYS:HE3	2.11	0.50
1:O:243:THR:HG21	1:O:273:TYR:CD2	2.46	0.50
1:H:351:VAL:CG1	1:H:369:HIS:HB3	2.41	0.50
1:P:41:THR:HB	1:P:44:GLU:HG3	1.94	0.50
1:C:38:MSE:CB	1:C:59:LEU:HD11	2.39	0.50
1:L:354:ARG:HH21	1:L:358:LEU:HD22	1.77	0.50
1:M:61:GLN:HA	1:M:64:GLN:HE21	1.75	0.50
1:H:467:ASN:HB3	1:H:471:PHE:HD2	1.76	0.50
1:P:120:CYS:O	1:P:175:TYR:HB3	2.10	0.50
1:N:347:LYS:HD3	1:N:357:SER:HB2	1.93	0.50
1:P:364:HIS:HB2	7:P:2053:HOH:O	2.11	0.50
1:I:152:GLU:CD	1:I:196:HIS:NE2	2.65	0.50
1:N:188:THR:HG21	1:N:195:PRO:HG3	1.92	0.50
1:L:127:PHE:O	1:L:128:ARG:NH1	2.42	0.50
1:E:24:LYS:HG2	1:E:25:GLY:H	1.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:VAL:CG1	1:E:507:LEU:HD22	2.41	0.50
1:D:61:GLN:HA	1:D:64:GLN:HE21	1.76	0.50
1:C:536:ARG:NE	1:H:333:SER:CB	2.74	0.50
1:B:429:THR:H	1:B:432:GLN:NE2	2.09	0.50
1:A:324:VAL:HG12	1:A:328:GLN:NE2	2.25	0.50
1:K:492:LEU:O	1:K:496:GLU:HG3	2.11	0.50
1:M:133:LEU:HB2	1:M:199:LEU:HD11	1.93	0.50
1:M:572:TRP:HA	7:M:2077:HOH:O	2.11	0.50
1:G:108:MSE:N	1:G:109:PRO:CD	2.75	0.50
1:O:332:VAL:HG22	1:O:336:GLU:HB2	1.93	0.50
1:A:386:PRO:O	1:A:407:MSE:HE3	2.12	0.50
1:J:466:ASN:HA	2:J:1581:NAP:N7N	2.17	0.50
1:H:92:ASN:C	1:H:92:ASN:ND2	2.58	0.50
1:A:133:LEU:HD22	1:A:135:ILE:HG13	1.93	0.50
1:E:168:GLY:O	1:E:425:LYS:HE2	2.12	0.50
1:K:352:LYS:NZ	1:K:352:LYS:HB3	2.27	0.50
1:H:137:ILE:HD13	1:H:226:ILE:HB	1.93	0.50
1:D:359:THR:HG22	1:D:361:GLU:N	2.21	0.50
1:G:227:ARG:NH1	1:G:227:ARG:HG3	2.25	0.50
1:G:359:THR:HG22	1:G:361:GLU:N	2.23	0.50
1:B:288:VAL:HG12	1:B:292:LEU:HD22	1.94	0.50
1:M:502:VAL:HG11	1:M:507:LEU:HD13	1.93	0.50
1:I:61:GLN:O	1:I:65:VAL:HG23	2.12	0.50
1:B:205:VAL:HG22	7:B:2016:HOH:O	2.10	0.50
1:M:532:LYS:HG2	1:M:549:LEU:HD12	1.93	0.50
1:P:58:PHE:N	5:P:1591:CL:CL	2.65	0.50
1:K:406:ASP:O	1:K:409:ALA:HB3	2.11	0.50
1:E:71:ASN:HB3	1:E:84:LEU:HD11	1.93	0.50
1:D:399:PHE:HB2	1:D:428:CYS:HB3	1.92	0.50
1:K:64:GLN:NE2	1:K:562:TYR:OH	2.42	0.50
1:E:177:MSE:O	1:E:180:PRO:HD2	2.12	0.50
1:F:270:ARG:HH11	1:F:270:ARG:HG2	1.77	0.50
1:B:285:SER:HB3	1:B:470:VAL:HG21	1.92	0.50
1:P:92:ASN:ND2	1:P:92:ASN:C	2.61	0.50
1:H:429:THR:CG2	1:H:430:ALA:N	2.75	0.50
1:H:140:ARG:HH12	1:H:230:ALA:CB	2.25	0.50
1:J:261:ASN:HA	1:J:264:ARG:NH1	2.27	0.50
1:K:92:ASN:C	1:K:92:ASN:HD22	2.15	0.50
1:D:165:ARG:HD2	1:D:165:ARG:O	2.10	0.50
1:L:504:GLU:O	1:L:508:GLN:HG3	2.12	0.50
1:A:543:TYR:HA	1:A:544:PRO:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:THR:HG22	1:F:137:ILE:N	2.27	0.50
1:I:533:GLU:CD	1:I:536:ARG:NH1	2.65	0.50
1:I:502:VAL:CG2	1:I:514:PRO:HD3	2.42	0.50
1:M:98:LYS:HD3	1:M:560:THR:HG21	1.93	0.50
1:P:350:ILE:HD13	1:P:362:LYS:HB3	1.94	0.50
1:E:183:LYS:HE3	1:E:255:GLU:CD	2.32	0.50
1:F:132:GLY:HA2	1:F:200:PRO:HG2	1.94	0.50
1:N:260:ALA:O	1:N:264:ARG:HG2	2.12	0.50
1:B:533:GLU:HG3	1:B:537:ASN:HD21	1.77	0.50
1:F:575:GLU:O	1:F:578:LYS:HG2	2.11	0.50
1:D:137:ILE:HA	1:D:234:LEU:HD22	1.93	0.50
1:C:138:HIS:NE2	1:C:223:HIS:HE1	2.10	0.49
1:C:433:LEU:HD12	1:C:443:PHE:HB2	1.93	0.49
1:P:381:VAL:CG1	1:P:407:MSE:HE1	2.42	0.49
1:D:136:THR:O	1:D:139:ASP:OD2	2.29	0.49
1:D:61:GLN:HE21	1:D:98:LYS:HE2	1.77	0.49
1:C:322:LEU:HD22	1:C:492:LEU:HD13	1.93	0.49
1:K:303:SER:HB3	1:K:332:VAL:HG21	1.94	0.49
1:P:243:THR:HG21	1:P:273:TYR:CD2	2.47	0.49
1:L:160:VAL:HG21	1:L:238:PHE:CE2	2.47	0.49
1:I:319:ILE:O	1:I:323:ILE:HG13	2.11	0.49
1:N:24:LYS:HD2	1:N:24:LYS:N	2.27	0.49
1:L:90:ASP:OD1	1:L:131:ARG:NH1	2.45	0.49
1:J:24:LYS:NZ	1:L:24:LYS:CD	2.75	0.49
1:C:328:GLN:HA	1:C:332:VAL:O	2.12	0.49
1:B:131:ARG:HD3	1:B:181:VAL:HG13	1.94	0.49
1:N:376:ASN:O	1:N:380:ILE:HG13	2.11	0.49
1:P:108:MSE:HB3	1:P:109:PRO:HD3	1.94	0.49
1:M:351:VAL:O	1:M:354:ARG:HB2	2.12	0.49
1:H:184:LEU:HD22	1:H:198:CYS:HB3	1.92	0.49
1:H:323:ILE:HG22	1:H:327:MSE:HE2	1.94	0.49
1:M:578:LYS:HZ2	1:M:580:LYS:N	2.10	0.49
1:E:429:THR:HB	1:E:432:GLN:HG3	1.94	0.49
1:O:381:VAL:CG1	1:O:407:MSE:HE1	2.40	0.49
1:M:148:GLN:CG	1:M:245:ARG:HH21	2.22	0.49
1:M:242:VAL:HG13	1:M:246:TYR:HD1	1.78	0.49
1:H:222:ARG:HG3	1:H:222:ARG:NH1	2.26	0.49
1:A:378:GLU:HA	1:A:403:ILE:CD1	2.42	0.49
1:L:183:LYS:HE3	1:L:255:GLU:CD	2.32	0.49
1:J:77:SER:O	1:J:81:ARG:HG3	2.12	0.49
1:D:301:ARG:HB3	1:D:330:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD22	1:A:399:PHE:CZ	2.48	0.49
1:I:136:THR:CG2	1:I:137:ILE:N	2.75	0.49
1:C:533:GLU:CD	1:C:536:ARG:NH1	2.66	0.49
1:B:428:CYS:HA	1:B:432:GLN:NE2	2.27	0.49
1:P:202:MSE:CE	1:P:203:LEU:C	2.81	0.49
1:P:164:GLU:HG2	1:P:258:ALA:HB2	1.94	0.49
1:E:165:ARG:HD2	1:E:165:ARG:O	2.11	0.49
1:P:500:GLN:HE21	1:P:500:GLN:CA	2.25	0.49
1:K:131:ARG:NH1	7:K:2013:HOH:O	2.45	0.49
1:O:302:LEU:HD22	1:O:327:MSE:HG3	1.93	0.49
1:F:429:THR:HG22	1:F:431:GLU:H	1.77	0.49
1:F:238:PHE:O	1:F:242:VAL:HG22	2.13	0.49
1:A:279:ASP:O	1:A:283:THR:HG21	2.13	0.49
1:P:202:MSE:CE	1:P:203:LEU:O	2.59	0.49
1:C:72:PHE:CZ	1:C:81:ARG:HD3	2.47	0.49
1:I:274:CYS:SG	1:I:478:VAL:HG11	2.53	0.49
1:O:340:ARG:HH11	1:O:340:ARG:HG2	1.77	0.49
1:D:467:ASN:ND2	3:D:1582:OXL:O2	2.46	0.49
1:A:184:LEU:O	1:A:187:TYR:HB2	2.13	0.49
1:K:154:VAL:CG1	1:K:154:VAL:O	2.60	0.49
1:D:61:GLN:HE21	1:D:98:LYS:CE	2.25	0.49
1:E:177:MSE:HE2	1:E:202:MSE:HB3	1.93	0.49
1:K:578:LYS:HE2	1:K:580:LYS:HB2	1.95	0.49
1:O:572:TRP:O	1:O:573:PRO:O	2.31	0.49
1:H:152:GLU:OE1	1:H:196:HIS:O	2.31	0.49
1:L:140:ARG:CD	7:L:2032:HOH:O	2.59	0.49
1:I:61:GLN:HE22	1:I:560:THR:HG23	1.78	0.49
1:N:317:LEU:HD23	1:N:343:MSE:HE1	1.94	0.49
1:I:141:GLY:H	1:I:237:GLU:CD	2.16	0.49
1:H:260:ALA:O	1:H:264:ARG:HG2	2.12	0.49
1:G:164:GLU:CG	1:G:258:ALA:HB2	2.33	0.49
1:A:359:THR:CG2	1:A:362:LYS:HE2	2.37	0.49
1:F:299:LYS:HZ3	1:F:299:LYS:HB3	1.73	0.49
1:C:429:THR:CG2	1:C:430:ALA:N	2.74	0.49
1:J:147:LEU:HB3	1:J:245:ARG:HD2	1.95	0.49
1:B:64:GLN:HB3	1:B:95:LEU:HD21	1.93	0.49
1:F:222:ARG:HD2	1:G:578:LYS:NZ	2.28	0.49
1:B:223:HIS:HD2	1:B:224:LYS:O	1.95	0.49
1:G:404:LEU:HD22	1:G:433:LEU:HD23	1.94	0.49
1:K:433:LEU:C	1:K:433:LEU:HD13	2.33	0.49
1:J:125:LEU:C	1:J:125:LEU:HD23	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:270:ARG:HH12	1:P:487:GLY:HA2	1.77	0.49
1:L:352:LYS:HG2	1:L:366:ALA:O	2.12	0.49
1:N:250:CYS:O	1:N:252:ILE:HD12	2.12	0.49
1:O:300:ASN:HB2	1:O:304:ASP:OD2	2.12	0.49
1:B:350:ILE:HD13	1:B:362:LYS:HB3	1.95	0.49
1:F:442:ILE:CG2	1:F:512:LEU:HD21	2.42	0.49
1:E:358:LEU:HD23	1:E:363:GLU:HG2	1.94	0.49
1:D:160:VAL:CG1	1:D:201:VAL:HB	2.22	0.49
1:H:361:GLU:N	1:H:361:GLU:OE1	2.45	0.49
1:J:108:MSE:HB3	1:J:109:PRO:HD3	1.95	0.49
1:D:152:GLU:OE1	1:D:196:HIS:CE1	2.66	0.49
1:J:354:ARG:HB3	1:J:358:LEU:CD2	2.40	0.49
1:J:166:ILE:HG21	1:J:172:LEU:HD12	1.95	0.49
1:N:207:THR:HA	1:N:225:ARG:HG2	1.94	0.49
1:H:132:GLY:HA2	1:H:200:PRO:HG2	1.95	0.49
1:H:133:LEU:HB2	1:H:199:LEU:HD11	1.95	0.49
1:I:406:ASP:HB3	1:I:410:PHE:CZ	2.47	0.49
1:M:470:VAL:HG13	1:M:494:THR:HG21	1.95	0.49
1:P:319:ILE:O	1:P:323:ILE:HG13	2.13	0.49
1:N:61:GLN:HG2	1:N:562:TYR:CE1	2.47	0.49
1:N:61:GLN:HE21	1:N:98:LYS:HE2	1.76	0.49
1:D:361:GLU:O	1:D:364:HIS:HB2	2.13	0.49
1:G:254:PHE:CE2	1:G:265:LEU:HD13	2.48	0.49
1:I:359:THR:HG22	1:I:362:LYS:CG	2.43	0.49
1:I:492:LEU:O	1:I:496:GLU:HG3	2.12	0.49
1:B:413:ARG:HH11	1:B:413:ARG:HG3	1.78	0.49
1:M:165:ARG:O	1:M:165:ARG:HD2	2.13	0.49
1:D:107:PHE:O	1:D:111:VAL:HG12	2.13	0.49
1:L:543:TYR:HA	1:L:544:PRO:C	2.33	0.49
1:B:154:VAL:O	1:B:154:VAL:HG13	2.12	0.49
1:K:575:GLU:HG2	1:K:576:ALA:N	2.28	0.49
1:L:327:MSE:HE1	1:L:337:ALA:O	2.12	0.48
1:P:284:ALA:HB1	1:P:322:LEU:HB2	1.95	0.48
1:H:416:ILE:HG13	1:H:433:LEU:CD2	2.37	0.48
1:P:428:CYS:HB2	1:P:432:GLN:HE21	1.77	0.48
1:O:250:CYS:O	1:O:252:ILE:HD12	2.13	0.48
1:O:48:LEU:HD11	1:O:565:PHE:HB3	1.95	0.48
1:F:239:MSE:HE1	1:F:252:ILE:HG21	1.94	0.48
1:G:243:THR:CG2	1:G:248:MSE:HA	2.42	0.48
1:K:467:ASN:ND2	3:K:1582:OXL:O2	2.46	0.48
1:I:533:GLU:OE2	1:I:536:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:OD1	1:A:95:LEU:HB2	2.12	0.48
1:E:401:GLN:HG2	1:E:436:TYR:CE2	2.48	0.48
1:J:172:LEU:O	1:J:175:TYR:HB2	2.13	0.48
1:B:92:ASN:C	1:B:92:ASN:HD22	2.15	0.48
1:G:220:GLY:HA2	1:H:56:PRO:HG2	1.95	0.48
1:G:232:ASP:OD1	1:G:264:ARG:NH2	2.40	0.48
1:D:172:LEU:O	1:D:175:TYR:HB2	2.13	0.48
1:O:158:ILE:HD12	1:O:242:VAL:HG11	1.94	0.48
1:J:429:THR:H	1:J:432:GLN:HG3	1.78	0.48
1:L:251:LEU:C	1:L:252:ILE:HD12	2.34	0.48
1:M:324:VAL:O	1:M:328:GLN:HG3	2.12	0.48
1:C:59:LEU:HD12	1:C:59:LEU:H	1.77	0.48
1:N:349:LEU:HB2	1:N:380:ILE:HD13	1.94	0.48
1:H:467:ASN:HB3	1:H:471:PHE:CD2	2.47	0.48
1:F:575:GLU:HG3	1:F:575:GLU:H	1.42	0.48
1:J:150:TRP:CE2	1:J:199:LEU:HD13	2.48	0.48
1:M:163:GLY:HA2	1:M:166:ILE:HD11	1.96	0.48
1:J:66:TYR:O	1:J:70:LYS:HG2	2.13	0.48
1:G:408:ALA:HB1	1:G:440:ARG:NH2	2.28	0.48
1:H:171:ASP:OD2	1:H:225:ARG:NH1	2.45	0.48
1:I:166:ILE:HA	1:I:256:ASP:OD1	2.13	0.48
1:E:221:LEU:HD13	1:E:223:HIS:CE1	2.48	0.48
1:O:328:GLN:HE22	1:O:334:LYS:NZ	2.11	0.48
1:L:104:ILE:CG1	1:L:108:MSE:HE3	2.37	0.48
1:M:24:LYS:HZ3	1:O:24:LYS:HE2	1.79	0.48
1:K:152:GLU:OE1	1:K:196:HIS:CE1	2.66	0.48
1:G:548:ASP:OD2	1:G:551:ALA:CB	2.60	0.48
1:I:23:LYS:HE2	1:I:27:GLU:HG2	1.95	0.48
1:C:207:THR:HA	1:C:225:ARG:HG2	1.95	0.48
1:A:165:ARG:HD2	1:A:165:ARG:C	2.34	0.48
1:E:36:LYS:HD2	1:E:562:TYR:HB3	1.96	0.48
1:H:167:LEU:HD23	1:H:422:PRO:HD3	1.94	0.48
1:I:570:TYR:H	1:K:46:GLN:HE22	1.61	0.48
1:K:471:PHE:CG	1:K:472:PRO:HD3	2.49	0.48
1:A:161:THR:HA	1:A:257:PHE:CE1	2.48	0.48
1:D:158:ILE:HD12	1:D:242:VAL:HG11	1.95	0.48
1:P:404:LEU:HD22	1:P:433:LEU:CD2	2.44	0.48
1:K:239:MSE:HE1	1:K:252:ILE:HG21	1.95	0.48
1:J:94:LYS:HD2	1:J:560:THR:O	2.12	0.48
1:G:227:ARG:HH11	1:G:227:ARG:CG	2.24	0.48
1:I:578:LYS:O	1:I:578:LYS:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:85:LEU:HD12	1:O:110:ILE:CG2	2.42	0.48
1:A:399:PHE:HB2	1:A:428:CYS:HB3	1.95	0.48
1:G:100:LEU:HD21	1:G:111:VAL:HG21	1.96	0.48
1:L:243:THR:HG21	1:L:273:TYR:CD2	2.49	0.48
1:F:543:TYR:HA	1:F:544:PRO:C	2.34	0.48
1:H:136:THR:CG2	1:H:137:ILE:N	2.76	0.48
1:A:41:THR:CG2	1:A:42:LEU:N	2.77	0.48
1:N:433:LEU:HG	1:N:443:PHE:HB2	1.94	0.48
1:D:572:TRP:O	1:D:577:MSE:HE2	2.13	0.48
1:E:238:PHE:CE2	1:E:239:MSE:HE3	2.48	0.48
1:F:350:ILE:HD13	1:F:362:LYS:HB3	1.94	0.48
1:J:556:GLN:NE2	1:J:556:GLN:CA	2.75	0.48
1:J:202:MSE:HE1	1:J:204:ASP:HA	1.94	0.48
1:B:254:PHE:CE2	1:B:265:LEU:HD13	2.47	0.48
1:O:579:VAL:HG23	1:O:579:VAL:O	2.14	0.48
1:L:245:ARG:HD3	1:L:246:TYR:CE2	2.48	0.48
1:O:125:LEU:N	5:O:1591:CL:CL	2.79	0.48
1:C:263:PHE:CZ	1:C:317:LEU:HD12	2.49	0.48
1:G:474:VAL:O	1:G:478:VAL:HG23	2.14	0.48
1:C:323:ILE:CG2	1:C:327:MSE:HE2	2.25	0.48
1:A:42:LEU:O	1:A:46:GLN:HG3	2.13	0.48
1:B:41:THR:O	1:B:45:ARG:HG3	2.13	0.48
1:E:250:CYS:O	1:E:252:ILE:HD12	2.14	0.48
1:G:377:LEU:O	1:G:381:VAL:HG23	2.13	0.48
1:C:536:ARG:HE	1:H:333:SER:HB2	1.79	0.48
1:C:270:ARG:CG	1:C:270:ARG:HH11	2.27	0.48
1:C:381:VAL:CG1	1:C:407:MSE:HE1	2.44	0.48
1:E:349:LEU:HB2	1:E:380:ILE:CD1	2.43	0.48
1:B:374:MSE:CE	1:B:379:ASP:HB3	2.43	0.48
1:O:369:HIS:HD1	1:O:370:CYS:N	2.12	0.48
1:F:240:GLU:O	1:F:244:SER:HB2	2.14	0.48
1:H:300:ASN:OD1	1:H:305:HIS:HE1	1.96	0.48
1:L:476:LEU:HD13	1:L:527:ALA:CB	2.43	0.48
1:A:215:ASP:O	1:A:222:ARG:NH2	2.47	0.48
1:G:196:HIS:HB3	7:G:2032:HOH:O	2.12	0.48
1:N:136:THR:CG2	1:N:137:ILE:N	2.76	0.48
1:K:136:THR:HG21	1:K:138:HIS:HB2	1.96	0.48
1:A:327:MSE:HE1	1:A:337:ALA:O	2.14	0.48
1:N:36:LYS:HE2	1:N:562:TYR:HB3	1.95	0.48
1:N:578:LYS:HZ1	1:O:222:ARG:HD3	1.79	0.48
1:D:572:TRP:C	1:D:573:PRO:O	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:VAL:HG12	1:E:507:LEU:CD2	2.44	0.48
1:N:350:ILE:HD13	1:N:362:LYS:HB3	1.94	0.48
1:C:92:ASN:ND2	1:C:95:LEU:H	2.11	0.48
1:I:208:ASP:OD1	1:I:225:ARG:HG3	2.13	0.48
1:B:202:MSE:HE3	1:B:203:LEU:N	2.28	0.48
1:B:177:MSE:O	1:B:180:PRO:HD2	2.13	0.48
1:B:295:LEU:HD11	1:B:302:LEU:HB2	1.96	0.48
1:K:302:LEU:HB3	1:K:330:GLU:OE1	2.14	0.48
1:J:188:THR:HG21	1:J:195:PRO:HG3	1.95	0.48
1:K:227:ARG:HH11	1:K:227:ARG:HG3	1.79	0.48
1:C:476:LEU:O	1:C:480:SER:HB2	2.13	0.48
1:B:85:LEU:HD12	1:B:110:ILE:HG21	1.96	0.48
1:L:281:GLN:HB3	1:L:491:PHE:CE1	2.48	0.48
1:A:117:GLY:O	1:A:121:GLN:HG3	2.14	0.48
1:O:327:MSE:HB3	1:O:332:VAL:CG1	2.42	0.48
1:N:61:GLN:HA	1:N:64:GLN:HE21	1.79	0.48
1:M:454:LEU:HD12	1:M:454:LEU:N	2.29	0.48
1:L:238:PHE:CE2	1:L:239:MSE:HE3	2.48	0.48
1:J:420:SER:HA	2:J:1581:NAP:H1D	1.95	0.48
1:K:250:CYS:O	1:K:252:ILE:HD12	2.14	0.48
1:E:283:THR:O	1:E:286:VAL:HG12	2.13	0.48
1:J:36:LYS:HD2	1:J:562:TYR:CG	2.49	0.48
1:G:77:SER:O	1:G:81:ARG:HG3	2.14	0.48
1:G:59:LEU:N	1:G:59:LEU:HD12	2.29	0.48
1:K:177:MSE:HE2	1:K:202:MSE:HB3	1.95	0.48
1:B:345:ASP:CG	1:B:354:ARG:HH22	2.16	0.48
1:H:502:VAL:CG1	1:H:507:LEU:HD13	2.44	0.48
1:D:343:MSE:HE3	1:D:365:PHE:CG	2.49	0.48
1:E:396:GLY:O	1:E:426:ALA:O	2.32	0.48
1:O:30:ARG:O	1:P:30:ARG:HD3	2.14	0.48
1:C:136:THR:HG22	1:C:137:ILE:N	2.27	0.48
1:P:133:LEU:HB3	1:P:201:VAL:HG22	1.95	0.48
1:L:104:ILE:CG1	1:L:108:MSE:CE	2.91	0.48
1:N:433:LEU:CD1	1:N:443:PHE:HB2	2.44	0.48
1:D:41:THR:HG22	1:D:43:GLU:N	2.20	0.48
1:N:314:GLU:HB2	2:N:1581:NAP:O1N	2.14	0.48
1:J:202:MSE:HE2	1:J:204:ASP:HB2	1.96	0.48
1:I:172:LEU:O	1:I:175:TYR:HB2	2.13	0.48
1:O:184:LEU:O	1:O:187:TYR:HB2	2.14	0.48
1:L:88:LEU:HD13	1:L:96:PHE:HA	1.96	0.48
1:B:417:PHE:CD1	1:B:444:ALA:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ARG:NH1	1:A:330:GLU:HG2	2.28	0.48
1:K:296:ARG:HB2	1:K:507:LEU:HD21	1.96	0.48
1:O:160:VAL:HG21	1:O:238:PHE:CE2	2.49	0.48
1:M:320:ALA:O	1:M:324:VAL:HG23	2.14	0.48
1:O:429:THR:CB	1:O:432:GLN:HG2	2.39	0.48
1:M:104:ILE:HG23	1:M:105:GLU:N	2.29	0.48
1:G:528:VAL:HG22	1:G:553:ILE:HD12	1.96	0.48
1:M:467:ASN:HD22	1:M:468:SER:N	2.11	0.48
1:J:183:LYS:HE3	1:J:255:GLU:OE1	2.14	0.48
1:I:104:ILE:CD1	1:I:108:MSE:HE3	2.42	0.48
1:J:152:GLU:HG3	1:J:155:ILE:HD12	1.96	0.48
1:M:374:MSE:HE1	1:M:379:ASP:O	2.14	0.48
1:P:113:THR:HG22	1:P:114:PRO:HA	1.94	0.48
1:O:543:TYR:HA	1:O:544:PRO:C	2.33	0.48
1:L:75:LEU:HD11	1:L:84:LEU:HD22	1.95	0.48
1:G:336:GLU:HG3	7:G:2038:HOH:O	2.13	0.48
1:A:260:ALA:HB3	7:A:2018:HOH:O	2.13	0.48
1:B:136:THR:CG2	1:B:137:ILE:N	2.77	0.47
1:L:136:THR:HG23	1:L:221:LEU:HD11	1.96	0.47
1:E:433:LEU:HD12	1:E:443:PHE:HB2	1.95	0.47
1:L:411:ASN:HB2	1:L:414:PRO:HG3	1.96	0.47
1:K:36:LYS:HG3	1:K:562:TYR:CG	2.49	0.47
1:C:86:MSE:CE	1:C:89:GLN:NE2	2.77	0.47
1:B:108:MSE:HE1	1:B:516:LEU:HG	1.96	0.47
1:B:429:THR:HG23	1:B:449:PHE:CE2	2.49	0.47
1:N:172:LEU:O	1:N:175:TYR:HB2	2.14	0.47
1:L:61:GLN:HA	1:L:64:GLN:HE21	1.79	0.47
1:K:429:THR:CG2	1:K:430:ALA:N	2.77	0.47
1:M:154:VAL:O	1:M:154:VAL:HG13	2.14	0.47
1:P:493:THR:O	1:P:497:VAL:HG23	2.14	0.47
1:K:172:LEU:HA	1:K:212:LEU:HD11	1.96	0.47
1:C:129:ARG:HG3	1:D:91:ARG:HD3	1.96	0.47
1:C:137:ILE:HB	1:C:205:VAL:HG12	1.95	0.47
1:O:108:MSE:N	1:O:109:PRO:CD	2.77	0.47
1:O:109:PRO:HA	1:O:113:THR:O	2.14	0.47
1:P:381:VAL:HG11	1:P:407:MSE:HE1	1.95	0.47
1:P:428:CYS:HB2	1:P:432:GLN:NE2	2.29	0.47
1:G:429:THR:CG2	1:G:430:ALA:N	2.76	0.47
1:G:243:THR:HG22	1:G:247:GLY:O	2.14	0.47
1:H:165:ARG:HD2	1:H:165:ARG:C	2.34	0.47
1:J:24:LYS:HZ2	1:L:24:LYS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:572:TRP:C	1:G:573:PRO:O	2.52	0.47
1:O:258:ALA:N	5:O:1589:CL:CL	2.76	0.47
1:K:529:ARG:NH1	1:K:529:ARG:HG2	2.28	0.47
1:P:500:GLN:HE21	1:P:500:GLN:N	2.13	0.47
1:K:56:PRO:HG2	1:L:220:GLY:HA2	1.96	0.47
1:I:112:TYR:CG	1:I:186:LEU:HD11	2.49	0.47
1:F:335:GLU:O	1:F:339:LYS:HG2	2.15	0.47
1:F:36:LYS:HD2	1:F:562:TYR:CG	2.49	0.47
1:G:296:ARG:HB2	1:G:507:LEU:HD21	1.96	0.47
1:B:61:GLN:HE22	1:B:560:THR:HG23	1.79	0.47
1:B:24:LYS:CE	1:D:24:LYS:HD3	2.44	0.47
1:K:64:GLN:HB3	1:K:95:LEU:CD2	2.44	0.47
1:E:133:LEU:HD23	1:E:134:PHE:N	2.29	0.47
1:H:78:ASP:HA	1:H:81:ARG:HH11	1.79	0.47
1:F:104:ILE:CG1	1:F:108:MSE:HE3	2.44	0.47
1:A:24:LYS:CD	1:A:24:LYS:O	2.63	0.47
1:F:375:LYS:HG2	7:F:2053:HOH:O	2.15	0.47
1:O:151:PRO:HG2	1:O:152:GLU:OE1	2.15	0.47
1:O:136:THR:CG2	1:O:137:ILE:N	2.77	0.47
1:E:433:LEU:HD13	1:E:433:LEU:C	2.35	0.47
1:H:433:LEU:HG	1:H:443:PHE:CD1	2.49	0.47
1:K:36:LYS:HE2	1:K:562:TYR:HB3	1.96	0.47
1:G:401:GLN:HA	1:G:436:TYR:CD2	2.50	0.47
1:F:210:GLU:OE2	1:F:224:LYS:HE2	2.14	0.47
1:J:467:ASN:HB3	1:J:471:PHE:HD2	1.80	0.47
1:D:429:THR:HB	1:D:432:GLN:HG3	1.96	0.47
1:M:300:ASN:OD1	1:M:305:HIS:CE1	2.67	0.47
1:A:229:GLN:HE21	1:A:229:GLN:CA	2.26	0.47
1:G:492:LEU:O	1:G:496:GLU:HG3	2.14	0.47
1:M:56:PRO:HG2	1:N:220:GLY:HA2	1.96	0.47
1:M:399:PHE:HB2	1:M:428:CYS:HB3	1.96	0.47
1:K:572:TRP:C	1:K:573:PRO:O	2.51	0.47
1:C:324:VAL:HA	1:C:327:MSE:HE3	1.95	0.47
1:M:433:LEU:HG	1:M:443:PHE:CB	2.38	0.47
1:A:316:ALA:HB1	1:A:343:MSE:HE1	1.93	0.47
1:F:239:MSE:CE	1:F:239:MSE:HA	2.40	0.47
1:I:354:ARG:HG2	1:I:356:ALA:N	2.30	0.47
1:C:431:GLU:OE2	1:C:452:VAL:HG22	2.14	0.47
1:E:402:GLN:CD	1:E:402:GLN:N	2.68	0.47
1:J:140:ARG:NH2	1:J:230:ALA:HA	2.30	0.47
1:J:41:THR:HG22	1:J:42:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:CD2	1:A:269:TYR:HE1	2.25	0.47
1:P:401:GLN:HG3	1:P:402:GLN:HE22	1.79	0.47
1:L:401:GLN:HB2	1:L:436:TYR:CE1	2.50	0.47
1:H:253:GLN:HE21	1:H:255:GLU:HG2	1.80	0.47
1:O:359:THR:OG1	1:O:360:PRO:HD2	2.14	0.47
1:C:578:LYS:HZ3	1:C:578:LYS:HB3	1.79	0.47
1:L:59:LEU:HD13	1:L:64:GLN:CG	2.44	0.47
1:F:72:PHE:CE1	1:F:81:ARG:HB3	2.50	0.47
1:C:356:ALA:HB2	1:I:230:ALA:CB	2.45	0.47
1:B:177:MSE:HG2	7:B:2012:HOH:O	2.14	0.47
1:I:59:LEU:HD13	1:I:64:GLN:HG2	1.96	0.47
1:F:125:LEU:C	1:F:125:LEU:HD13	2.35	0.47
1:C:554:ARG:NH1	1:C:554:ARG:HG2	2.29	0.47
1:C:402:GLN:NE2	1:C:402:GLN:H	2.11	0.47
1:K:24:LYS:HA	1:K:28:VAL:HG23	1.96	0.47
1:H:321:ASN:HB2	7:H:2041:HOH:O	2.14	0.47
1:M:36:LYS:HD2	1:M:562:TYR:HB3	1.96	0.47
1:B:543:TYR:HA	1:B:544:PRO:C	2.35	0.47
1:H:376:ASN:O	1:H:380:ILE:HG13	2.14	0.47
1:M:429:THR:CG2	1:M:430:ALA:N	2.77	0.47
1:N:59:LEU:HA	1:P:580:LYS:H	1.79	0.47
1:H:327:MSE:HE3	1:H:337:ALA:CB	2.31	0.47
1:K:401:GLN:HG3	1:K:436:TYR:CG	2.50	0.47
1:G:72:PHE:CE2	1:G:81:ARG:HD3	2.50	0.47
1:I:207:THR:HA	1:I:225:ARG:HG2	1.96	0.47
1:B:296:ARG:CB	1:B:507:LEU:HD21	2.44	0.47
1:P:162:ASP:O	1:P:225:ARG:NH2	2.30	0.47
1:H:467:ASN:ND2	3:H:1582:OXL:O2	2.48	0.47
1:D:309:PHE:HB2	1:D:343:MSE:HG2	1.96	0.47
1:I:469:TYR:OH	1:I:516:LEU:HD13	2.14	0.47
1:L:146:MSE:O	1:L:149:SER:HB3	2.15	0.47
1:C:315:ALA:O	1:C:319:ILE:HG13	2.15	0.47
1:E:61:GLN:O	1:E:65:VAL:HG23	2.14	0.47
1:C:56:PRO:HG2	1:D:220:GLY:HA2	1.96	0.47
1:O:471:PHE:CG	1:O:472:PRO:HD3	2.49	0.47
1:N:399:PHE:HB2	1:N:428:CYS:HB3	1.95	0.47
1:M:136:THR:CG2	1:M:138:HIS:N	2.72	0.47
1:K:381:VAL:HG13	1:K:407:MSE:HE1	1.96	0.47
1:L:158:ILE:HD12	1:L:242:VAL:HG11	1.95	0.47
1:M:578:LYS:NZ	1:M:580:LYS:CD	2.78	0.47
1:M:23:LYS:O	1:M:24:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:THR:CG2	1:D:42:LEU:N	2.77	0.47
1:D:404:LEU:HD22	1:D:433:LEU:HD23	1.96	0.47
1:J:270:ARG:NH1	1:J:270:ARG:CG	2.75	0.47
1:O:270:ARG:CG	1:O:270:ARG:HH11	2.28	0.47
1:E:162:ASP:HA	1:E:202:MSE:CE	2.44	0.47
1:B:420:SER:HA	2:B:1581:NAP:HD1D	1.96	0.47
1:I:467:ASN:HD22	1:I:468:SER:N	2.12	0.47
1:A:352:LYS:HA	1:A:352:LYS:HD3	1.68	0.47
1:K:385:LYS:HA	1:K:410:PHE:HE2	1.79	0.47
1:G:288:VAL:HG21	1:G:322:LEU:CD1	2.45	0.47
1:F:494:THR:HG23	1:F:526:ILE:CG2	2.42	0.47
1:H:431:GLU:HG2	1:H:452:VAL:HG22	1.97	0.47
1:H:155:ILE:HD13	1:H:246:TYR:CE2	2.50	0.47
1:C:245:ARG:HH11	1:C:245:ARG:HG2	1.80	0.47
1:G:36:LYS:HD2	1:G:562:TYR:CG	2.49	0.47
1:N:86:MSE:HE1	1:N:89:GLN:NE2	2.30	0.47
1:M:133:LEU:HD23	1:N:52:GLY:O	2.14	0.47
1:D:285:SER:HB3	1:D:470:VAL:HG21	1.97	0.47
1:I:166:ILE:HG21	1:I:172:LEU:HD12	1.97	0.47
1:K:23:LYS:C	1:K:24:LYS:HD2	2.35	0.47
1:B:459:THR:HG22	1:B:461:TYR:CE1	2.49	0.47
1:L:36:LYS:NZ	1:L:44:GLU:OE1	2.46	0.47
1:M:548:ASP:OD2	1:M:551:ALA:HB2	2.15	0.47
1:D:23:LYS:HB3	1:D:23:LYS:HE2	1.63	0.47
1:K:239:MSE:HE1	1:K:252:ILE:HG12	1.97	0.47
1:D:41:THR:HG22	1:D:42:LEU:N	2.28	0.47
1:E:164:GLU:CG	1:E:258:ALA:HB2	2.44	0.47
1:J:354:ARG:NE	1:J:358:LEU:HD21	2.30	0.47
1:A:254:PHE:HE2	1:A:265:LEU:HD13	1.80	0.47
1:B:165:ARG:NH1	2:B:1581:NAP:O1N	2.47	0.47
1:J:59:LEU:O	1:J:59:LEU:HD12	2.15	0.47
1:L:301:ARG:HG3	7:L:2040:HOH:O	2.15	0.47
1:E:61:GLN:HA	1:E:64:GLN:HE21	1.79	0.47
1:B:195:PRO:HD2	7:B:2015:HOH:O	2.15	0.47
1:K:135:ILE:HD12	1:K:135:ILE:N	2.30	0.47
1:F:90:ASP:OD1	1:F:131:ARG:NH1	2.48	0.47
1:O:396:GLY:O	1:O:426:ALA:O	2.32	0.47
1:D:369:HIS:ND1	1:D:370:CYS:O	2.41	0.47
1:B:23:LYS:HG2	1:B:24:LYS:N	2.30	0.47
1:K:404:LEU:HD13	1:K:433:LEU:HA	1.95	0.47
1:J:359:THR:HG22	1:J:362:LYS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:420:SER:HA	2:K:1581:NAP:H1D	1.96	0.47
1:H:314:GLU:HB2	2:H:1581:NAP:O1N	2.15	0.47
1:I:74:ARG:HD3	1:J:125:LEU:HD21	1.96	0.47
1:K:315:ALA:O	1:K:319:ILE:HG13	2.14	0.47
1:C:354:ARG:HD2	1:C:356:ALA:N	2.30	0.47
1:I:61:GLN:HA	1:I:64:GLN:HE21	1.79	0.47
1:P:109:PRO:HA	1:P:113:THR:O	2.15	0.47
1:B:471:PHE:CE1	1:B:472:PRO:HG3	2.50	0.47
1:C:274:CYS:SG	1:C:478:VAL:HG11	2.55	0.47
1:O:575:GLU:O	1:O:578:LYS:HB3	2.15	0.47
1:E:41:THR:O	1:E:45:ARG:HG3	2.15	0.47
1:K:476:LEU:HB3	1:K:527:ALA:HB2	1.96	0.47
1:H:332:VAL:CG1	1:H:336:GLU:HB2	2.45	0.47
1:L:209:ASN:OD1	1:L:211:THR:HB	2.15	0.47
1:B:243:THR:HG21	1:B:273:TYR:CD2	2.50	0.47
1:A:359:THR:CG2	1:A:362:LYS:HG3	2.44	0.47
1:I:323:ILE:O	1:I:327:MSE:HG3	2.15	0.47
1:D:35:ASN:HD21	1:D:37:GLY:H	1.56	0.47
1:E:162:ASP:HA	1:E:202:MSE:HE1	1.98	0.47
1:N:88:LEU:HD13	1:N:96:PHE:HA	1.96	0.47
1:I:374:MSE:CE	1:I:379:ASP:HB3	2.44	0.47
1:O:317:LEU:HD23	1:O:343:MSE:HE1	1.96	0.47
1:O:33:HIS:HD2	1:O:93:GLU:OE2	1.98	0.47
1:L:152:GLU:HG2	1:L:196:HIS:O	2.15	0.47
1:O:145:THR:O	1:O:148:GLN:HB2	2.15	0.47
1:A:274:CYS:SG	1:A:478:VAL:HG11	2.54	0.47
1:L:137:ILE:HA	1:L:234:LEU:HD22	1.97	0.46
1:L:420:SER:HA	2:L:1581:NAP:H1D	1.96	0.46
1:F:24:LYS:HG2	1:H:24:LYS:NZ	2.29	0.46
1:I:77:SER:HB2	1:I:80:ASP:OD2	2.14	0.46
1:A:135:ILE:HB	1:A:203:LEU:HD23	1.97	0.46
1:L:60:GLY:O	1:L:64:GLN:HG3	2.15	0.46
1:C:359:THR:HG23	1:C:360:PRO:HD2	1.97	0.46
1:K:77:SER:O	1:K:81:ARG:HG3	2.14	0.46
1:K:556:GLN:HE21	1:K:556:GLN:CA	2.28	0.46
1:N:165:ARG:HD2	1:N:165:ARG:O	2.15	0.46
1:P:467:ASN:HB3	1:P:471:PHE:HD2	1.80	0.46
1:L:574:GLU:OE1	1:L:577:MSE:HE2	2.15	0.46
1:H:374:MSE:CE	1:H:379:ASP:HB3	2.44	0.46
1:P:158:ILE:HD12	1:P:242:VAL:HG11	1.97	0.46
1:H:433:LEU:HD13	1:H:433:LEU:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:THR:HG22	1:G:431:GLU:H	1.79	0.46
1:N:104:ILE:HG23	1:N:105:GLU:N	2.30	0.46
1:C:89:GLN:HG3	1:C:96:PHE:CD2	2.50	0.46
1:G:202:MSE:CE	1:G:204:ASP:HA	2.46	0.46
1:D:504:GLU:HG3	1:D:508:GLN:HE21	1.78	0.46
1:F:78:ASP:HA	1:F:81:ARG:HH11	1.81	0.46
1:B:529:ARG:NH1	1:B:529:ARG:HG2	2.30	0.46
1:B:113:THR:CG2	1:B:114:PRO:HA	2.44	0.46
1:F:154:VAL:HG13	1:F:154:VAL:O	2.15	0.46
1:I:154:VAL:HG13	1:I:154:VAL:O	2.14	0.46
1:N:368:GLU:O	1:N:368:GLU:HG3	2.15	0.46
1:D:575:GLU:OE2	1:D:576:ALA:HB2	2.14	0.46
1:F:467:ASN:ND2	3:F:1582:OXL:O2	2.48	0.46
1:N:184:LEU:HD22	1:N:198:CYS:HB3	1.96	0.46
1:O:328:GLN:CD	1:O:334:LYS:HD2	2.35	0.46
1:I:354:ARG:HG2	1:I:356:ALA:H	1.79	0.46
1:E:288:VAL:HG12	1:E:292:LEU:HD13	1.98	0.46
1:P:162:ASP:HA	1:P:202:MSE:CE	2.45	0.46
1:K:359:THR:HG22	1:K:362:LYS:CD	2.45	0.46
1:N:160:VAL:HG12	1:N:161:THR:N	2.30	0.46
1:K:58:PHE:N	1:K:58:PHE:CD1	2.83	0.46
1:L:321:ASN:HB2	7:L:2044:HOH:O	2.13	0.46
1:E:543:TYR:HA	1:E:544:PRO:C	2.35	0.46
1:E:476:LEU:O	1:E:480:SER:HB2	2.15	0.46
1:O:328:GLN:HE22	1:O:334:LYS:HD2	1.77	0.46
1:P:433:LEU:HG	1:P:443:PHE:CD1	2.50	0.46
1:F:239:MSE:HE1	1:F:252:ILE:HD13	1.97	0.46
1:O:428:CYS:HB2	1:O:432:GLN:HE21	1.80	0.46
1:D:381:VAL:HG13	1:D:407:MSE:HE1	1.97	0.46
1:B:381:VAL:CG1	1:B:407:MSE:HE1	2.46	0.46
1:C:533:GLU:OE1	1:C:536:ARG:NH1	2.48	0.46
1:C:161:THR:HG22	1:C:180:PRO:HG2	1.96	0.46
1:O:350:ILE:HD11	1:O:362:LYS:HD2	1.98	0.46
1:F:264:ARG:NH1	1:F:264:ARG:HG2	2.28	0.46
1:L:152:GLU:HB3	1:L:155:ILE:HD11	1.98	0.46
1:H:98:LYS:HD3	1:H:560:THR:CG2	2.45	0.46
1:I:70:LYS:HA	1:I:70:LYS:HD3	1.78	0.46
1:M:86:MSE:HE1	1:M:89:GLN:NE2	2.31	0.46
1:F:202:MSE:HE3	1:F:204:ASP:HA	1.98	0.46
1:P:407:MSE:O	1:P:411:ASN:HB2	2.15	0.46
1:M:24:LYS:HB2	1:M:24:LYS:HZ2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:MSE:CE	1:O:177:MSE:CA	2.91	0.46
1:J:108:MSE:N	1:J:109:PRO:CD	2.79	0.46
1:N:164:GLU:CG	1:N:258:ALA:HB2	2.40	0.46
1:G:44:GLU:O	1:G:48:LEU:HB2	2.16	0.46
1:B:391:GLY:HA3	1:B:427:GLU:HG2	1.97	0.46
1:A:202:MSE:HE2	1:A:204:ASP:HA	1.97	0.46
1:F:108:MSE:HB3	1:F:109:PRO:HD3	1.97	0.46
1:A:89:GLN:HB2	1:A:96:PHE:CE1	2.51	0.46
1:B:192:GLY:HA3	1:B:557:VAL:HG13	1.96	0.46
1:K:179:ILE:HB	1:K:180:PRO:HD3	1.96	0.46
1:C:404:LEU:HD22	1:C:433:LEU:HD23	1.96	0.46
1:D:324:VAL:HG12	1:D:328:GLN:NE2	2.21	0.46
1:E:340:ARG:HH11	1:E:340:ARG:CG	2.29	0.46
1:L:314:GLU:HB2	2:L:1581:NAP:O1N	2.16	0.46
1:L:454:LEU:CD2	1:L:460:LEU:HG	2.42	0.46
1:A:215:ASP:OD1	1:A:216:PRO:HD2	2.16	0.46
1:G:335:GLU:OE2	1:G:339:LYS:NZ	2.44	0.46
1:C:554:ARG:HH11	1:C:554:ARG:HG2	1.79	0.46
1:N:476:LEU:HB3	1:N:527:ALA:HB2	1.98	0.46
1:J:192:GLY:HA3	1:J:557:VAL:HG13	1.98	0.46
1:D:376:ASN:O	1:D:380:ILE:HG13	2.15	0.46
1:A:91:ARG:HB3	1:A:91:ARG:HE	1.49	0.46
1:P:376:ASN:O	1:P:380:ILE:HG13	2.15	0.46
1:G:123:TYR:HB3	1:G:175:TYR:CD2	2.51	0.46
1:A:188:THR:OG1	1:A:195:PRO:HG3	2.16	0.46
1:L:323:ILE:HG22	1:L:327:MSE:HE2	1.98	0.46
1:P:407:MSE:HG2	1:P:416:ILE:HD11	1.97	0.46
1:O:239:MSE:HE1	1:O:252:ILE:HG21	1.97	0.46
1:B:160:VAL:HG21	1:B:238:PHE:CE2	2.50	0.46
1:B:238:PHE:CE2	1:B:239:MSE:HE3	2.50	0.46
1:L:131:ARG:O	1:L:177:MSE:HE3	2.16	0.46
1:E:202:MSE:HE3	1:E:203:LEU:C	2.35	0.46
1:D:524:LEU:O	1:D:528:VAL:HG23	2.16	0.46
1:M:270:ARG:HG2	1:M:270:ARG:HH11	1.80	0.46
1:N:177:MSE:O	1:N:180:PRO:HD2	2.16	0.46
1:C:108:MSE:HB3	1:C:109:PRO:HD3	1.97	0.46
1:B:332:VAL:HG12	1:B:333:SER:N	2.30	0.46
1:P:155:ILE:HB	1:P:246:TYR:CE2	2.51	0.46
1:D:458:GLN:HE21	1:D:460:LEU:HD21	1.80	0.46
1:K:543:TYR:HA	1:K:544:PRO:C	2.35	0.46
1:A:172:LEU:O	1:A:175:TYR:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:385:LYS:HA	1:P:410:PHE:CE2	2.51	0.46
1:E:90:ASP:OD1	1:E:131:ARG:NH1	2.48	0.46
1:K:378:GLU:OE2	1:K:382:LYS:NZ	2.46	0.46
1:D:416:ILE:CG1	1:D:433:LEU:HD21	2.39	0.46
1:M:92:ASN:ND2	1:M:92:ASN:C	2.58	0.46
1:K:410:PHE:CD1	1:K:410:PHE:N	2.84	0.46
1:B:578:LYS:O	1:B:578:LYS:HD2	2.15	0.46
1:O:92:ASN:ND2	1:O:92:ASN:C	2.69	0.46
1:C:284:ALA:HA	1:C:319:ILE:HG12	1.97	0.46
1:A:175:TYR:CE2	1:A:218:TYR:HA	2.51	0.46
1:N:69:LEU:HD22	1:N:106:ARG:HH12	1.79	0.46
1:M:516:LEU:HA	1:M:516:LEU:HD12	1.75	0.46
1:E:342:TRP:CD2	1:E:367:HIS:HD2	2.34	0.46
1:A:404:LEU:HD22	1:A:433:LEU:HD23	1.98	0.46
1:P:327:MSE:O	1:P:332:VAL:HG12	2.16	0.46
1:K:164:GLU:CG	1:K:258:ALA:HB2	2.38	0.46
1:G:254:PHE:HE2	1:G:265:LEU:HD13	1.81	0.46
1:E:283:THR:CG2	1:E:284:ALA:N	2.79	0.46
1:J:41:THR:CG2	7:J:2006:HOH:O	2.64	0.46
1:C:141:GLY:N	1:C:237:GLU:OE1	2.39	0.46
1:C:580:LYS:HG3	1:C:580:LYS:O	2.15	0.46
1:P:502:VAL:CG1	1:P:507:LEU:HD13	2.46	0.46
1:K:184:LEU:HD12	1:K:200:PRO:HB3	1.97	0.46
1:A:332:VAL:CG1	1:A:333:SER:N	2.79	0.46
1:B:35:ASN:ND2	1:B:37:GLY:H	2.14	0.46
1:G:177:MSE:O	1:G:180:PRO:HD2	2.16	0.46
1:L:414:PRO:HD2	1:L:441:GLY:HA2	1.98	0.46
1:K:407:MSE:HG2	1:K:416:ILE:HD11	1.98	0.46
1:M:578:LYS:HZ1	1:M:580:LYS:CD	2.26	0.46
1:J:137:ILE:HA	1:J:234:LEU:HD22	1.97	0.46
1:I:222:ARG:HD2	1:L:580:LYS:CE	2.45	0.46
1:K:288:VAL:HG21	1:K:322:LEU:HB3	1.98	0.46
1:A:64:GLN:O	1:A:68:ILE:HG12	2.15	0.46
1:B:59:LEU:N	1:B:59:LEU:HD12	2.30	0.46
1:G:61:GLN:HA	1:G:64:GLN:HE21	1.80	0.46
1:K:454:LEU:CD1	1:K:454:LEU:N	2.79	0.46
1:H:351:VAL:HG12	1:H:369:HIS:HB3	1.97	0.46
1:K:516:LEU:O	1:K:519:ILE:HG22	2.16	0.46
1:B:222:ARG:HH11	1:B:222:ARG:HG3	1.80	0.46
1:D:159:VAL:HG23	1:D:184:LEU:HD21	1.98	0.46
1:J:47:GLN:NE2	1:J:566:VAL:HG13	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:543:TYR:HA	1:P:544:PRO:C	2.36	0.46
1:B:120:CYS:O	1:B:175:TYR:HB3	2.16	0.46
1:F:103:ASP:HB3	1:F:107:PHE:CE1	2.50	0.46
1:A:476:LEU:HB3	1:A:527:ALA:HB2	1.97	0.46
1:P:524:LEU:O	1:P:528:VAL:HG23	2.15	0.46
1:P:580:LYS:HB3	1:P:580:LYS:HE2	1.58	0.45
1:H:386:PRO:CG	1:H:407:MSE:HE1	2.33	0.45
1:O:381:VAL:HG13	1:O:407:MSE:CE	2.41	0.45
1:C:38:MSE:SE	1:C:55:PRO:HG2	2.66	0.45
1:C:132:GLY:HA2	1:C:200:PRO:HG2	1.98	0.45
1:P:572:TRP:C	1:P:573:PRO:O	2.54	0.45
1:I:108:MSE:N	1:I:109:PRO:CD	2.79	0.45
1:B:415:ILE:CG1	1:B:442:ILE:HD12	2.46	0.45
1:O:74:ARG:HD3	1:P:125:LEU:HD21	1.98	0.45
1:K:38:MSE:SE	1:K:57:CYS:SG	3.24	0.45
1:G:36:LYS:HD3	1:G:562:TYR:HB3	1.98	0.45
1:G:257:PHE:O	1:G:314:GLU:OE2	2.35	0.45
1:F:184:LEU:HD12	1:F:200:PRO:HB3	1.97	0.45
1:G:502:VAL:HG12	1:G:507:LEU:HD13	1.98	0.45
1:C:165:ARG:HD2	1:C:165:ARG:O	2.15	0.45
1:I:117:GLY:O	1:I:121:GLN:HG3	2.16	0.45
1:E:184:LEU:HD22	1:E:198:CYS:HB3	1.98	0.45
1:H:145:THR:HA	1:H:148:GLN:NE2	2.30	0.45
1:K:470:VAL:HG13	1:K:494:THR:HG21	1.97	0.45
1:L:296:ARG:O	1:L:299:LYS:HE3	2.15	0.45
1:F:291:LEU:HD21	1:F:388:VAL:HG11	1.98	0.45
1:G:133:LEU:HB2	1:G:199:LEU:HD11	1.98	0.45
1:I:369:HIS:ND1	1:I:370:CYS:N	2.63	0.45
1:C:41:THR:CG2	1:C:43:GLU:H	2.30	0.45
1:I:322:LEU:HD23	1:I:322:LEU:HA	1.76	0.45
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.75	0.45
7:J:2027:HOH:O	1:K:580:LYS:HD2	2.15	0.45
1:N:202:MSE:HE1	1:N:204:ASP:HA	1.99	0.45
1:A:229:GLN:HA	1:A:229:GLN:HE21	1.81	0.45
1:A:91:ARG:HB2	1:B:129:ARG:HH12	1.81	0.45
1:H:35:ASN:ND2	1:H:37:GLY:H	2.14	0.45
1:E:309:PHE:HB2	1:E:343:MSE:HG2	1.98	0.45
1:C:433:LEU:O	1:C:437:THR:HG23	2.17	0.45
1:P:389:LEU:HD22	1:P:399:PHE:CZ	2.51	0.45
1:C:23:LYS:O	1:C:24:LYS:HG3	2.16	0.45
1:M:324:VAL:HA	1:M:327:MSE:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:GLN:HB3	1:K:95:LEU:HD21	1.97	0.45
1:L:354:ARG:NE	1:L:358:LEU:HD21	2.32	0.45
1:I:163:GLY:HA2	1:I:166:ILE:HD11	1.97	0.45
1:H:108:MSE:N	1:H:109:PRO:CD	2.78	0.45
1:L:578:LYS:HB3	1:L:578:LYS:HE2	1.82	0.45
1:G:152:GLU:OE2	1:G:154:VAL:HG13	2.17	0.45
1:A:156:LYS:HD3	1:A:479:ILE:HG23	1.98	0.45
1:A:214:LYS:HD3	7:A:2015:HOH:O	2.15	0.45
1:A:33:HIS:HD2	1:A:93:GLU:OE2	1.97	0.45
1:L:117:GLY:O	1:L:121:GLN:HG3	2.15	0.45
1:F:36:LYS:CD	1:F:562:TYR:HB3	2.47	0.45
1:M:427:GLU:O	1:M:428:CYS:HB3	2.17	0.45
1:A:194:LYS:HA	1:A:195:PRO:HD3	1.87	0.45
1:D:184:LEU:O	1:D:187:TYR:HB2	2.17	0.45
1:D:543:TYR:HA	1:D:544:PRO:C	2.36	0.45
1:K:376:ASN:O	1:K:380:ILE:HG13	2.16	0.45
1:N:253:GLN:NE2	1:N:255:GLU:OE1	2.47	0.45
1:M:543:TYR:HA	1:M:544:PRO:C	2.36	0.45
1:I:136:THR:CG2	1:I:221:LEU:HD11	2.47	0.45
1:M:136:THR:OG1	1:M:221:LEU:HD11	2.17	0.45
1:C:42:LEU:O	1:C:46:GLN:HG3	2.16	0.45
1:A:466:ASN:HA	2:A:1581:NAP:N7N	2.20	0.45
1:A:316:ALA:HB1	1:A:343:MSE:HE2	1.96	0.45
1:N:572:TRP:C	1:N:573:PRO:O	2.54	0.45
1:M:378:GLU:OE1	1:M:382:LYS:HE2	2.15	0.45
1:N:44:GLU:O	1:N:48:LEU:HB2	2.15	0.45
1:L:120:CYS:O	1:L:175:TYR:HB3	2.16	0.45
1:M:88:LEU:CD1	1:M:96:PHE:HA	2.46	0.45
1:M:36:LYS:HE2	1:M:40:PHE:CD2	2.52	0.45
1:C:204:ASP:HA	7:C:2026:HOH:O	2.16	0.45
1:M:161:THR:HA	1:M:257:PHE:CE1	2.52	0.45
1:C:174:CYS:SG	1:C:219:ILE:CD1	3.04	0.45
1:H:543:TYR:HA	1:H:544:PRO:C	2.37	0.45
1:G:136:THR:HG23	1:G:221:LEU:HD11	1.99	0.45
1:D:328:GLN:HA	1:D:332:VAL:O	2.17	0.45
1:K:467:ASN:N	2:K:1581:NAP:H72N	2.15	0.45
1:F:350:ILE:HG22	1:F:350:ILE:O	2.17	0.45
1:A:429:THR:HG22	1:A:430:ALA:H	1.82	0.45
1:P:98:LYS:HD3	1:P:560:THR:CG2	2.47	0.45
1:G:77:SER:HB2	1:G:80:ASP:OD2	2.17	0.45
1:A:401:GLN:HG2	1:A:436:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:162:ASP:HA	1:P:202:MSE:HE1	1.98	0.45
1:G:64:GLN:NE2	1:G:562:TYR:OH	2.50	0.45
1:O:340:ARG:HG2	1:O:340:ARG:NH1	2.32	0.45
1:A:82:TYR:CE2	1:A:86:MSE:HG3	2.51	0.45
1:P:276:PHE:HB2	1:P:281:GLN:OE1	2.17	0.45
1:D:435:LYS:HE3	1:D:436:TYR:CE1	2.52	0.45
1:B:535:TYR:HE2	1:B:549:LEU:HD21	1.81	0.45
1:L:300:ASN:OD1	1:L:305:HIS:HE1	1.99	0.45
1:C:494:THR:CG2	1:C:526:ILE:HD12	2.25	0.45
1:A:469:TYR:OH	1:A:516:LEU:HD12	2.17	0.45
1:L:454:LEU:HD22	1:L:454:LEU:H	1.81	0.45
1:J:402:GLN:HG3	7:J:2041:HOH:O	2.17	0.45
1:K:245:ARG:HG2	1:K:245:ARG:NH1	2.32	0.45
1:K:359:THR:HG22	1:K:362:LYS:CG	2.47	0.45
1:O:571:THR:HG23	1:O:572:TRP:N	2.32	0.45
1:D:429:THR:H	1:D:432:GLN:NE2	2.15	0.45
1:O:120:CYS:O	1:O:175:TYR:HB3	2.16	0.45
1:N:309:PHE:HB2	1:N:343:MSE:HG2	1.98	0.45
1:L:243:THR:HG21	1:L:273:TYR:HD2	1.81	0.45
1:P:222:ARG:HH11	1:P:222:ARG:HG3	1.82	0.45
1:C:32:PRO:HD2	1:D:30:ARG:NH2	2.32	0.45
1:E:260:ALA:O	1:E:264:ARG:HG2	2.16	0.45
1:H:412:LYS:O	1:H:413:ARG:HD2	2.17	0.45
1:D:90:ASP:OD2	1:D:131:ARG:NH1	2.50	0.45
1:N:138:HIS:NE2	1:N:223:HIS:CE1	2.83	0.45
1:J:429:THR:HG22	1:J:431:GLU:N	2.30	0.45
1:J:61:GLN:HE21	1:J:98:LYS:HE2	1.82	0.45
1:P:454:LEU:HD21	1:P:460:LEU:CD1	2.44	0.45
1:N:350:ILE:HG23	1:N:358:LEU:CD1	2.47	0.45
1:H:427:GLU:CD	1:H:427:GLU:H	2.19	0.45
1:L:68:ILE:HD13	7:L:2009:HOH:O	2.17	0.45
1:C:312:ALA:CB	1:C:362:LYS:HE2	2.47	0.45
1:C:252:ILE:HD12	1:C:252:ILE:N	2.32	0.45
1:F:33:HIS:HD2	1:F:93:GLU:OE2	2.00	0.45
1:E:112:TYR:CG	1:E:186:LEU:HD11	2.52	0.45
1:N:493:THR:HG23	1:N:529:ARG:NH1	2.32	0.45
1:A:456:SER:HB3	7:A:2023:HOH:O	2.16	0.45
1:I:399:PHE:HB2	1:I:428:CYS:HB3	1.98	0.45
1:A:470:VAL:HG13	1:A:494:THR:HG21	1.99	0.45
1:A:136:THR:CG2	1:A:137:ILE:N	2.80	0.45
1:H:61:GLN:O	1:H:65:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:GLU:HB2	2:K:1581:NAP:O1N	2.17	0.45
1:I:359:THR:HG22	1:I:362:LYS:HG3	1.98	0.45
1:K:288:VAL:HG12	1:K:292:LEU:HD22	1.98	0.45
1:O:357:SER:C	1:O:358:LEU:HD12	2.35	0.45
1:O:189:ALA:O	1:O:520:GLN:NE2	2.41	0.45
1:I:376:ASN:O	1:I:380:ILE:HG13	2.16	0.45
1:L:442:ILE:HG22	1:L:512:LEU:HD11	1.99	0.45
1:P:132:GLY:HA2	1:P:200:PRO:HG2	1.98	0.45
1:H:483:LEU:HD12	1:H:539:THR:HB	1.99	0.45
1:D:160:VAL:HG11	1:D:238:PHE:CZ	2.51	0.45
1:L:137:ILE:HB	1:L:205:VAL:HG12	1.98	0.45
1:H:359:THR:HG23	1:H:361:GLU:N	2.31	0.45
1:M:578:LYS:NZ	1:M:580:LYS:CA	2.79	0.45
1:J:319:ILE:O	1:J:323:ILE:HG13	2.17	0.45
1:H:284:ALA:O	1:H:288:VAL:HG23	2.17	0.45
1:N:108:MSE:N	1:N:109:PRO:CD	2.80	0.45
1:A:270:ARG:HH11	1:A:270:ARG:HG2	1.81	0.45
1:G:528:VAL:CG1	1:G:532:LYS:HE2	2.47	0.45
1:L:183:LYS:NZ	1:L:467:ASN:ND2	2.65	0.45
1:M:529:ARG:NH1	1:M:529:ARG:HG2	2.32	0.45
1:C:556:GLN:CA	1:C:556:GLN:HE21	2.29	0.45
1:E:343:MSE:HE3	1:E:365:PHE:CG	2.51	0.45
1:L:285:SER:HB3	1:L:470:VAL:HG21	1.98	0.45
1:G:454:LEU:HB3	1:G:455:PRO:HD2	1.99	0.45
1:H:327:MSE:HE1	1:H:337:ALA:O	2.17	0.44
1:E:305:HIS:O	1:E:340:ARG:NH1	2.50	0.44
1:O:146:MSE:HE3	1:P:51:HIS:NE2	2.31	0.44
1:P:61:GLN:HE21	1:P:98:LYS:HE3	1.82	0.44
1:I:533:GLU:HG3	1:I:537:ASN:HD21	1.80	0.44
1:D:529:ARG:HD2	1:D:529:ARG:HA	1.81	0.44
1:H:324:VAL:HG12	1:H:328:GLN:HE21	1.81	0.44
1:N:494:THR:HG23	1:N:526:ILE:HD13	1.98	0.44
1:G:335:GLU:HG3	1:G:336:GLU:N	2.33	0.44
1:K:209:ASN:OD1	1:K:211:THR:HB	2.17	0.44
1:M:132:GLY:HA2	1:M:200:PRO:HG2	1.98	0.44
1:M:162:ASP:O	1:M:225:ARG:NH2	2.39	0.44
1:M:368:GLU:HG3	7:M:2044:HOH:O	2.17	0.44
1:K:220:GLY:HA2	1:L:56:PRO:HG2	1.98	0.44
1:E:420:SER:HA	2:E:1581:NAP:H1D	1.99	0.44
1:P:429:THR:CG2	1:P:430:ALA:N	2.80	0.44
1:A:42:LEU:CD2	1:C:577:MSE:HE3	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:SER:O	1:G:340:ARG:CZ	2.66	0.44
1:J:476:LEU:HD23	1:J:476:LEU:O	2.18	0.44
1:C:322:LEU:HD21	1:C:492:LEU:HB2	2.00	0.44
1:B:332:VAL:HG13	1:B:336:GLU:HB3	1.98	0.44
1:O:572:TRP:C	1:O:573:PRO:O	2.55	0.44
1:K:331:GLY:HA3	1:O:300:ASN:HA	1.98	0.44
1:K:24:LYS:N	1:K:24:LYS:HD2	2.32	0.44
1:P:33:HIS:HD2	1:P:93:GLU:OE2	2.00	0.44
1:B:276:PHE:HB2	1:B:281:GLN:OE1	2.16	0.44
1:O:327:MSE:HE1	1:O:341:ILE:CD1	2.47	0.44
1:K:154:VAL:C	1:K:155:ILE:HD12	2.37	0.44
1:M:95:LEU:O	1:M:99:VAL:HG23	2.17	0.44
1:C:133:LEU:HB2	1:C:199:LEU:HD11	1.98	0.44
1:J:401:GLN:O	1:J:405:GLN:HB2	2.18	0.44
1:B:162:ASP:C	1:B:202:MSE:HE1	2.37	0.44
1:A:378:GLU:HA	1:A:403:ILE:HD13	1.99	0.44
1:B:92:ASN:ND2	1:B:92:ASN:C	2.70	0.44
1:O:94:LYS:HD3	1:O:558:TYR:OH	2.18	0.44
1:A:261:ASN:OD1	1:A:264:ARG:NH1	2.49	0.44
1:G:33:HIS:HD2	1:G:93:GLU:OE2	2.00	0.44
1:M:222:ARG:HH11	1:M:222:ARG:HG3	1.83	0.44
1:P:429:THR:HG23	7:P:2064:HOH:O	2.17	0.44
1:L:466:ASN:HA	2:L:1581:NAP:N7N	2.24	0.44
1:D:284:ALA:HA	1:D:319:ILE:HG12	2.00	0.44
1:F:227:ARG:HD3	7:F:2045:HOH:O	2.16	0.44
1:D:61:GLN:HE22	1:D:560:THR:HG23	1.83	0.44
1:B:389:LEU:CD1	1:B:407:MSE:HE3	2.44	0.44
1:F:92:ASN:C	1:F:92:ASN:ND2	2.68	0.44
1:B:332:VAL:CG1	1:B:333:SER:N	2.80	0.44
1:O:110:ILE:O	1:O:115:THR:HB	2.18	0.44
1:N:470:VAL:O	1:N:474:VAL:HG23	2.17	0.44
1:D:401:GLN:HG3	1:D:436:TYR:CD1	2.53	0.44
1:C:192:GLY:HA3	1:C:557:VAL:HG13	2.00	0.44
1:H:104:ILE:HG23	1:H:105:GLU:N	2.31	0.44
1:M:30:ARG:O	1:N:30:ARG:HD3	2.16	0.44
1:P:35:ASN:ND2	1:P:37:GLY:H	2.14	0.44
1:C:261:ASN:O	1:C:265:LEU:HG	2.18	0.44
1:O:429:THR:H	1:O:432:GLN:HG3	1.83	0.44
1:L:35:ASN:HD21	1:L:37:GLY:H	1.60	0.44
1:E:283:THR:HG23	1:E:284:ALA:N	2.33	0.44
1:F:23:LYS:C	1:F:24:LYS:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:O	1:A:288:VAL:HG23	2.17	0.44
1:K:284:ALA:HA	1:K:319:ILE:HG12	1.98	0.44
1:K:284:ALA:HB1	1:K:322:LEU:HB2	1.99	0.44
1:K:429:THR:HG23	1:K:449:PHE:CD2	2.52	0.44
1:N:415:ILE:HG12	1:N:442:ILE:HD12	1.99	0.44
1:P:227:ARG:HG3	1:P:227:ARG:NH1	2.31	0.44
1:O:285:SER:HB3	1:O:470:VAL:HG21	1.99	0.44
1:C:154:VAL:HG13	1:C:154:VAL:O	2.17	0.44
1:P:340:ARG:NH1	1:P:340:ARG:HG2	2.32	0.44
1:B:100:LEU:HD21	1:B:111:VAL:HG21	1.99	0.44
1:A:57:CYS:HB3	1:B:219:ILE:O	2.18	0.44
1:K:188:THR:OG1	1:K:195:PRO:HG3	2.17	0.44
1:K:300:ASN:HD22	1:K:304:ASP:HB2	1.82	0.44
1:P:136:THR:CG2	1:P:137:ILE:N	2.80	0.44
1:H:359:THR:CG2	1:H:361:GLU:HB2	2.48	0.44
1:O:158:ILE:HG12	1:O:199:LEU:HB3	1.99	0.44
1:A:358:LEU:CD2	1:A:363:GLU:HG3	2.39	0.44
1:O:41:THR:HG21	7:O:2006:HOH:O	2.18	0.44
1:B:301:ARG:HH11	1:B:301:ARG:CB	2.26	0.44
1:L:41:THR:CG2	1:L:42:LEU:N	2.81	0.44
1:G:467:ASN:HB3	1:G:471:PHE:HD2	1.83	0.44
1:C:92:ASN:C	1:C:92:ASN:ND2	2.71	0.44
1:L:61:GLN:HG3	1:L:562:TYR:CE1	2.52	0.44
1:J:33:HIS:HD2	1:J:93:GLU:OE1	1.98	0.44
1:N:401:GLN:HG2	1:N:436:TYR:CZ	2.53	0.44
1:C:556:GLN:CA	1:C:556:GLN:NE2	2.80	0.44
1:O:471:PHE:CD1	1:O:472:PRO:HD3	2.52	0.44
1:E:184:LEU:O	1:E:187:TYR:HB2	2.18	0.44
1:I:165:ARG:NH2	1:I:279:ASP:OD1	2.48	0.44
1:B:572:TRP:C	1:B:573:PRO:O	2.54	0.44
1:F:324:VAL:O	1:F:328:GLN:HG3	2.18	0.44
1:C:172:LEU:O	1:C:175:TYR:HB2	2.17	0.44
1:B:433:LEU:C	1:B:433:LEU:HD13	2.37	0.44
1:F:429:THR:HG23	1:F:449:PHE:CE2	2.53	0.44
1:M:578:LYS:HZ1	1:M:580:LYS:CB	2.22	0.44
1:E:133:LEU:HB3	1:E:201:VAL:HG22	1.98	0.44
1:G:399:PHE:CD1	1:G:399:PHE:N	2.86	0.44
1:C:533:GLU:HG3	1:C:537:ASN:HD21	1.83	0.44
1:C:507:LEU:HD12	1:C:507:LEU:HA	1.79	0.44
1:G:61:GLN:NE2	1:G:98:LYS:HD3	2.33	0.44
1:B:188:THR:HG21	1:B:195:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:LEU:HB3	1:E:527:ALA:HB2	1.98	0.44
1:A:172:LEU:HA	1:A:212:LEU:HD11	2.00	0.44
1:K:159:VAL:HG23	1:K:184:LEU:HD21	2.00	0.44
1:I:110:ILE:O	1:I:115:THR:HB	2.18	0.44
1:L:266:LEU:O	1:L:270:ARG:HB2	2.18	0.44
1:A:151:PRO:HG2	1:A:152:GLU:OE1	2.17	0.44
1:O:284:ALA:HA	1:O:319:ILE:HG12	2.00	0.44
1:I:401:GLN:HG3	1:I:402:GLN:NE2	2.33	0.44
1:O:160:VAL:HG12	1:O:161:THR:N	2.32	0.44
1:O:36:LYS:HD2	1:O:562:TYR:CG	2.53	0.44
1:F:227:ARG:CG	1:F:227:ARG:NH1	2.79	0.44
1:D:152:GLU:OE1	1:D:196:HIS:NE2	2.51	0.44
1:L:401:GLN:HB2	1:L:436:TYR:CG	2.53	0.44
1:B:165:ARG:O	1:B:256:ASP:HB3	2.17	0.44
1:C:177:MSE:HG2	1:C:202:MSE:CG	2.47	0.44
1:I:578:LYS:HE3	1:I:580:LYS:HB2	2.00	0.44
1:J:381:VAL:HG13	1:J:407:MSE:HE1	2.00	0.44
1:C:351:VAL:O	1:C:354:ARG:HB2	2.18	0.44
1:L:172:LEU:O	1:L:175:TYR:HB2	2.18	0.44
1:H:123:TYR:HB3	1:H:175:TYR:CD2	2.52	0.44
1:L:399:PHE:HB2	1:L:428:CYS:HB3	2.00	0.44
1:I:401:GLN:HB2	1:I:436:TYR:CD1	2.53	0.44
1:N:50:ILE:HA	1:N:53:LEU:HD12	1.99	0.44
1:P:264:ARG:HG3	1:P:265:LEU:N	2.31	0.44
1:K:66:TYR:C	1:K:66:TYR:CD1	2.91	0.44
1:P:274:CYS:SG	1:P:478:VAL:HG11	2.58	0.44
1:P:516:LEU:O	1:P:519:ILE:HG22	2.18	0.44
1:K:137:ILE:HD13	1:K:226:ILE:HB	2.00	0.44
1:L:138:HIS:NE2	1:L:223:HIS:HE1	2.16	0.44
1:E:433:LEU:CD1	1:E:443:PHE:HB2	2.47	0.44
1:P:433:LEU:C	1:P:433:LEU:HD13	2.38	0.44
1:A:570:TYR:CE2	1:D:142:HIS:CG	3.06	0.44
1:O:41:THR:CG2	1:O:42:LEU:N	2.80	0.44
1:J:312:ALA:HB3	1:J:362:LYS:HE2	1.98	0.44
1:E:315:ALA:O	1:E:319:ILE:HG13	2.17	0.44
1:F:46:GLN:OE1	1:H:569:SER:HA	2.18	0.44
1:M:145:THR:O	1:M:148:GLN:HB2	2.17	0.44
1:G:327:MSE:HE2	1:G:337:ALA:HA	2.00	0.44
1:J:184:LEU:O	1:J:187:TYR:HB2	2.17	0.44
1:F:327:MSE:HE1	1:F:337:ALA:O	2.17	0.44
1:G:572:TRP:O	1:G:577:MSE:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:ALA:O	1:G:319:ILE:HG13	2.18	0.44
1:D:120:CYS:O	1:D:175:TYR:HB3	2.18	0.44
1:N:471:PHE:CG	1:N:472:PRO:HD3	2.52	0.44
1:H:296:ARG:O	1:H:299:LYS:NZ	2.51	0.44
1:O:154:VAL:HG22	1:O:154:VAL:O	2.18	0.44
1:I:162:ASP:C	1:I:162:ASP:OD1	2.57	0.44
1:G:493:THR:HG23	1:G:529:ARG:NH1	2.33	0.44
1:G:251:LEU:HD23	1:G:274:CYS:SG	2.58	0.44
1:B:324:VAL:HG12	1:B:328:GLN:HE21	1.83	0.44
1:H:394:ALA:HA	1:H:420:SER:HB3	1.99	0.44
1:A:342:TRP:CE2	1:A:384:ILE:HD12	2.53	0.44
1:E:77:SER:HB3	1:E:80:ASP:OD2	2.18	0.44
1:B:24:LYS:CD	1:D:24:LYS:NZ	2.81	0.43
1:L:108:MSE:N	1:L:109:PRO:CD	2.81	0.43
1:F:350:ILE:CD1	1:F:362:LYS:HD3	2.43	0.43
1:D:152:GLU:HB3	1:D:155:ILE:HD11	2.00	0.43
1:L:42:LEU:O	1:L:46:GLN:HG3	2.17	0.43
1:I:416:ILE:CG1	1:I:433:LEU:HD21	2.46	0.43
1:N:270:ARG:NH1	1:N:270:ARG:HG2	2.30	0.43
1:M:478:VAL:HG13	1:M:483:LEU:HB3	2.00	0.43
1:G:471:PHE:CG	1:G:472:PRO:HD3	2.53	0.43
1:F:108:MSE:HE2	1:F:190:CYS:SG	2.58	0.43
1:B:123:TYR:HB3	1:B:175:TYR:CD2	2.53	0.43
1:F:100:LEU:HD23	1:F:107:PHE:HB3	1.99	0.43
1:M:33:HIS:HD2	1:M:93:GLU:OE2	2.00	0.43
1:F:354:ARG:HG2	1:F:356:ALA:H	1.81	0.43
1:M:164:GLU:HG2	1:M:258:ALA:HB2	1.99	0.43
1:I:334:LYS:O	1:I:338:ILE:HG13	2.18	0.43
1:K:74:ARG:HD3	1:L:125:LEU:HD11	2.00	0.43
1:N:389:LEU:HD22	1:N:399:PHE:CZ	2.52	0.43
1:G:136:THR:CG2	1:G:137:ILE:N	2.81	0.43
1:J:314:GLU:HB2	2:J:1581:NAP:O1N	2.18	0.43
1:H:160:VAL:HG21	1:H:238:PHE:CE2	2.52	0.43
1:B:165:ARG:O	1:B:165:ARG:NE	2.49	0.43
1:J:24:LYS:CD	1:L:24:LYS:HD2	2.48	0.43
1:K:359:THR:HG22	1:K:362:LYS:HG3	2.00	0.43
1:F:554:ARG:HG2	1:F:554:ARG:NH1	2.32	0.43
1:A:165:ARG:O	1:A:256:ASP:HB3	2.18	0.43
1:H:157:ALA:HB2	1:H:479:ILE:HD11	1.99	0.43
1:N:557:VAL:HG12	1:N:558:TYR:N	2.33	0.43
1:N:85:LEU:HD12	1:N:110:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ALA:HA	1:F:319:ILE:HG12	2.00	0.43
1:E:132:GLY:CA	1:E:200:PRO:HG2	2.47	0.43
1:C:174:CYS:HB2	1:C:220:GLY:HA3	1.99	0.43
1:E:412:LYS:O	1:E:413:ARG:HD2	2.18	0.43
1:P:530:ILE:HG12	7:P:2072:HOH:O	2.19	0.43
1:J:516:LEU:H	1:J:516:LEU:HD22	1.82	0.43
1:H:268:LYS:HG2	1:H:269:TYR:CE2	2.52	0.43
1:O:327:MSE:HE1	1:O:341:ILE:HD11	2.00	0.43
1:C:404:LEU:HD13	1:C:433:LEU:HA	2.00	0.43
1:B:41:THR:CG2	1:B:42:LEU:N	2.81	0.43
1:K:196:HIS:HB2	7:K:2017:HOH:O	2.18	0.43
1:D:359:THR:HG23	1:D:360:PRO:CD	2.44	0.43
1:I:41:THR:CG2	1:I:42:LEU:N	2.81	0.43
1:K:322:LEU:HD21	1:K:492:LEU:HB2	2.00	0.43
1:O:165:ARG:C	1:O:165:ARG:HD2	2.39	0.43
1:H:156:LYS:HD2	1:H:197:GLN:OE1	2.19	0.43
1:H:266:LEU:O	1:H:270:ARG:HB2	2.18	0.43
1:K:172:LEU:O	1:K:175:TYR:HB2	2.18	0.43
1:I:374:MSE:HE1	1:I:379:ASP:HB3	1.99	0.43
1:H:98:LYS:HD3	1:H:560:THR:HG21	2.00	0.43
1:B:166:ILE:HG21	1:B:172:LEU:HD12	2.01	0.43
1:L:529:ARG:HH11	1:L:529:ARG:HG3	1.82	0.43
1:P:82:TYR:CE2	1:P:86:MSE:HG3	2.53	0.43
1:C:413:ARG:HD2	7:C:2047:HOH:O	2.18	0.43
1:B:171:ASP:OD2	1:B:225:ARG:HD2	2.19	0.43
1:O:104:ILE:CG1	1:O:108:MSE:CE	2.92	0.43
1:F:428:CYS:HA	1:F:432:GLN:HE22	1.84	0.43
1:B:23:LYS:HG2	1:B:24:LYS:H	1.82	0.43
1:H:322:LEU:HD23	1:H:322:LEU:HA	1.88	0.43
1:D:573:PRO:O	1:D:577:MSE:HE2	2.19	0.43
1:L:483:LEU:CD1	1:L:539:THR:HB	2.44	0.43
1:J:507:LEU:HD13	1:J:511:ARG:O	2.18	0.43
1:B:428:CYS:CB	1:B:432:GLN:HE21	2.31	0.43
1:K:245:ARG:NH1	7:K:2015:HOH:O	2.50	0.43
1:B:303:SER:HB2	1:B:332:VAL:HG21	1.98	0.43
1:P:38:MSE:HE3	5:P:1589:CL:CL	2.55	0.43
1:A:229:GLN:NE2	1:A:229:GLN:CA	2.81	0.43
1:G:375:LYS:HB2	1:G:375:LYS:HE3	1.89	0.43
1:J:374:MSE:CE	1:J:379:ASP:HB3	2.49	0.43
1:G:334:LYS:O	1:G:338:ILE:HG13	2.18	0.43
1:N:245:ARG:HG2	1:N:246:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:THR:HB	1:F:139:ASP:OD2	2.18	0.43
1:F:177:MSE:HE2	1:F:180:PRO:HD2	2.01	0.43
1:B:98:LYS:HD3	1:B:560:THR:HG23	1.99	0.43
1:L:165:ARG:NH2	2:L:1581:NAP:O1N	2.50	0.43
1:A:429:THR:CG2	1:A:430:ALA:H	2.30	0.43
1:D:155:ILE:HD13	1:D:246:TYR:CZ	2.53	0.43
1:D:98:LYS:HD3	1:D:560:THR:HG23	1.99	0.43
1:A:104:ILE:HD11	1:A:108:MSE:CE	2.48	0.43
1:C:166:ILE:HG23	1:C:179:ILE:HG13	2.00	0.43
1:B:429:THR:H	1:B:432:GLN:HE21	1.66	0.43
1:A:401:GLN:HG2	1:A:436:TYR:CD1	2.53	0.43
1:K:387:THR:HG22	1:K:411:ASN:OD1	2.18	0.43
1:P:177:MSE:HE2	1:P:202:MSE:HB3	2.00	0.43
1:O:78:ASP:HA	1:O:81:ARG:NH1	2.34	0.43
1:H:194:LYS:HD2	1:H:197:GLN:HE22	1.83	0.43
1:A:91:ARG:HB2	1:B:129:ARG:NH1	2.34	0.43
1:E:529:ARG:HG2	1:E:529:ARG:HH11	1.82	0.43
1:C:471:PHE:CG	1:C:472:PRO:HD3	2.54	0.43
1:A:406:ASP:HB3	1:A:410:PHE:CZ	2.54	0.43
1:P:388:VAL:HG22	1:P:415:ILE:HB	2.00	0.43
1:C:63:ALA:O	1:C:66:TYR:HB3	2.18	0.43
1:O:494:THR:HG23	1:O:526:ILE:HD13	2.00	0.43
1:L:374:MSE:HE1	1:L:379:ASP:C	2.39	0.43
1:F:188:THR:OG1	1:F:195:PRO:HG3	2.17	0.43
1:O:515:PRO:HG2	5:O:1588:CL:CL	2.56	0.43
1:E:215:ASP:O	1:E:222:ARG:NH2	2.49	0.43
1:B:136:THR:CG2	1:B:221:LEU:HD11	2.45	0.43
1:E:137:ILE:HA	1:E:234:LEU:CD2	2.47	0.43
1:O:137:ILE:HA	1:O:234:LEU:HD22	1.99	0.43
1:B:352:LYS:CE	1:B:353:GLY:N	2.80	0.43
1:N:578:LYS:HE3	1:N:580:LYS:HB2	2.01	0.43
1:N:322:LEU:HD23	1:N:322:LEU:HA	1.83	0.43
1:O:71:ASN:OD1	1:P:125:LEU:HD23	2.19	0.43
1:F:420:SER:HA	2:F:1581:NAP:H1D	2.01	0.43
1:H:309:PHE:HB2	1:H:343:MSE:HG2	2.01	0.43
1:N:86:MSE:CE	1:N:89:GLN:NE2	2.81	0.43
1:K:120:CYS:O	1:K:175:TYR:HB3	2.19	0.43
1:C:174:CYS:HB3	1:C:219:ILE:HD12	2.00	0.43
1:N:117:GLY:O	1:N:121:GLN:HG3	2.18	0.43
1:E:445:SER:HG	1:E:449:PHE:HD1	1.61	0.43
1:C:117:GLY:O	1:C:121:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:ILE:O	1:K:108:MSE:HB2	2.18	0.43
1:H:442:ILE:HG22	1:H:512:LEU:HD11	2.01	0.43
1:G:26:TYR:HE1	1:G:30:ARG:NH1	2.17	0.43
1:J:570:TYR:OH	1:K:139:ASP:HB3	2.19	0.43
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.48	0.43
1:A:394:ALA:HB2	2:A:1581:NAP:O3D	2.18	0.43
1:D:135:ILE:HB	1:D:203:LEU:HD23	1.99	0.43
1:B:467:ASN:O	1:B:470:VAL:N	2.41	0.43
1:K:165:ARG:C	1:K:165:ARG:HD2	2.39	0.43
1:N:536:ARG:CG	1:N:536:ARG:HH11	2.32	0.43
1:C:174:CYS:SG	1:C:219:ILE:HD12	2.58	0.43
1:P:340:ARG:HG2	1:P:340:ARG:HH11	1.83	0.43
1:P:516:LEU:HD12	1:P:516:LEU:HA	1.81	0.43
1:N:392:VAL:O	1:N:392:VAL:HG23	2.18	0.43
1:I:245:ARG:HH11	1:I:245:ARG:CG	2.31	0.43
1:J:512:LEU:HA	1:J:512:LEU:HD23	1.86	0.43
1:H:229:GLN:HG3	1:H:233:ASP:OD2	2.18	0.43
1:P:100:LEU:HD21	1:P:111:VAL:HG21	2.01	0.43
1:D:86:MSE:HE1	1:D:89:GLN:NE2	2.34	0.43
1:O:218:TYR:HB3	1:O:222:ARG:HH12	1.83	0.43
1:J:164:GLU:OE2	1:J:227:ARG:NH2	2.52	0.43
1:E:374:MSE:CE	1:E:379:ASP:HB3	2.48	0.43
1:C:285:SER:HB3	1:C:470:VAL:HG21	2.00	0.43
1:F:521:GLN:HE22	1:F:554:ARG:HH22	1.66	0.43
1:B:413:ARG:NH1	1:B:413:ARG:HG3	2.34	0.43
1:B:36:LYS:H	1:B:40:PHE:HE1	1.65	0.43
1:B:77:SER:O	1:B:81:ARG:HG3	2.18	0.43
1:J:165:ARG:C	1:J:165:ARG:HD2	2.39	0.43
1:O:172:LEU:O	1:O:175:TYR:HB2	2.18	0.43
1:N:215:ASP:HA	1:N:216:PRO:HD2	1.92	0.43
1:N:210:GLU:HA	1:N:213:LEU:HD12	1.99	0.43
1:K:352:LYS:HD3	1:K:368:GLU:HG2	2.00	0.43
1:D:376:ASN:HB3	1:D:379:ASP:OD2	2.18	0.43
1:E:56:PRO:HG2	1:F:220:GLY:HA2	2.01	0.43
1:O:58:PHE:CD1	1:O:58:PHE:N	2.86	0.43
1:K:534:ALA:HA	1:K:539:THR:OG1	2.19	0.43
1:G:56:PRO:HG2	1:H:220:GLY:HA2	2.01	0.43
1:E:274:CYS:SG	1:E:478:VAL:HG11	2.59	0.43
1:F:286:VAL:HG22	1:F:513:TYR:CE2	2.54	0.43
1:K:79:LEU:HD13	1:K:118:LEU:CD1	2.48	0.43
1:D:516:LEU:O	1:D:519:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:THR:O	1:L:224:LYS:HA	2.19	0.43
1:G:164:GLU:HB2	1:G:225:ARG:NH2	2.34	0.43
1:H:61:GLN:HG3	1:H:562:TYR:CE1	2.54	0.43
1:E:284:ALA:HA	1:E:319:ILE:HG12	2.01	0.43
1:O:385:LYS:HE3	1:O:410:PHE:CD1	2.53	0.43
1:C:148:GLN:HA	1:C:245:ARG:HH21	1.84	0.43
1:N:160:VAL:HG21	1:N:238:PHE:HE2	1.84	0.43
1:O:305:HIS:CD2	1:O:387:THR:OG1	2.72	0.43
1:F:545:GLN:HA	1:F:546:PRO:HD3	1.87	0.43
1:M:417:PHE:CD1	1:M:444:ALA:HB3	2.54	0.43
1:G:448:PRO:HD3	1:G:464:GLN:NE2	2.33	0.43
1:D:243:THR:HG21	1:D:273:TYR:CD2	2.54	0.43
1:G:105:GLU:HG2	1:G:516:LEU:HD23	2.01	0.43
1:D:239:MSE:HE1	1:D:252:ILE:HG21	2.01	0.43
1:O:59:LEU:HB2	1:O:63:ALA:HB3	2.01	0.43
1:E:284:ALA:O	1:E:288:VAL:HG23	2.18	0.43
1:B:78:ASP:HA	1:B:81:ARG:HH11	1.84	0.43
1:J:92:ASN:ND2	1:J:92:ASN:C	2.72	0.43
1:H:167:LEU:HB3	1:H:168:GLY:H	1.67	0.43
1:E:466:ASN:HA	2:E:1581:NAP:H72N	1.83	0.43
1:O:174:CYS:SG	1:O:219:ILE:HD12	2.59	0.43
1:B:245:ARG:HG2	1:B:246:TYR:CE2	2.54	0.43
1:E:136:THR:CG2	1:E:221:LEU:HD11	2.49	0.42
1:C:497:VAL:CG1	1:C:526:ILE:HD13	2.48	0.42
1:A:404:LEU:HD22	1:A:433:LEU:CD2	2.49	0.42
1:G:376:ASN:OD1	1:G:378:GLU:N	2.52	0.42
1:D:359:THR:CG2	1:D:360:PRO:HD2	2.47	0.42
1:E:166:ILE:HG23	1:E:179:ILE:HG13	2.01	0.42
1:A:516:LEU:O	1:A:519:ILE:HG22	2.19	0.42
1:C:177:MSE:O	1:C:180:PRO:HD2	2.19	0.42
1:D:47:GLN:HE22	1:D:566:VAL:CG1	2.32	0.42
1:J:402:GLN:CD	1:J:402:GLN:N	2.72	0.42
1:M:467:ASN:H	2:M:1581:NAP:H72N	1.67	0.42
1:M:471:PHE:CG	1:M:472:PRO:HD3	2.54	0.42
1:P:202:MSE:HE2	1:P:203:LEU:C	2.40	0.42
1:L:500:GLN:HE21	1:L:500:GLN:CA	2.31	0.42
1:P:59:LEU:HB2	1:P:63:ALA:HB3	2.01	0.42
1:L:467:ASN:ND2	3:L:1582:OXL:O2	2.51	0.42
1:B:39:ALA:CB	1:B:562:TYR:CE1	3.02	0.42
1:O:210:GLU:HG2	7:O:2040:HOH:O	2.18	0.42
1:O:354:ARG:HG3	1:O:373:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:467:ASN:ND2	3:P:1582:OXL:O2	2.52	0.42
1:F:100:LEU:HD23	1:F:107:PHE:CB	2.49	0.42
1:C:261:ASN:HA	1:C:264:ARG:NH1	2.34	0.42
1:A:492:LEU:O	1:A:496:GLU:HG3	2.19	0.42
1:P:554:ARG:HG2	1:P:554:ARG:HH11	1.84	0.42
1:F:164:GLU:HG2	1:F:258:ALA:HB2	2.01	0.42
1:E:471:PHE:N	1:E:472:PRO:CD	2.82	0.42
1:D:140:ARG:NH1	1:D:230:ALA:HA	2.34	0.42
1:N:152:GLU:CD	1:N:196:HIS:NE2	2.73	0.42
1:H:359:THR:HG22	1:H:362:LYS:N	2.15	0.42
1:E:323:ILE:HG22	1:E:327:MSE:HE2	2.01	0.42
1:A:136:THR:HG23	1:A:137:ILE:N	2.34	0.42
1:M:319:ILE:O	1:M:323:ILE:HG13	2.19	0.42
1:J:359:THR:HG22	1:J:362:LYS:HG3	2.00	0.42
1:B:431:GLU:OE1	1:B:452:VAL:HG13	2.19	0.42
1:A:315:ALA:O	1:A:319:ILE:HG13	2.20	0.42
1:E:546:PRO:HB2	1:E:549:LEU:HD23	2.01	0.42
1:F:113:THR:CG2	1:F:114:PRO:HA	2.49	0.42
1:J:303:SER:O	1:J:340:ARG:CZ	2.67	0.42
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.84	0.42
1:F:132:GLY:CA	1:F:200:PRO:HG2	2.49	0.42
1:J:78:ASP:HA	1:J:81:ARG:HH11	1.83	0.42
1:F:442:ILE:HG21	1:F:512:LEU:HD21	2.00	0.42
1:H:162:ASP:O	1:H:225:ARG:NH2	2.52	0.42
1:A:408:ALA:HB1	1:A:440:ARG:HH22	1.84	0.42
1:F:153:SER:HA	1:F:245:ARG:HH12	1.84	0.42
1:A:388:VAL:HG22	1:A:415:ILE:HB	2.00	0.42
1:B:61:GLN:HE21	1:B:98:LYS:NZ	2.17	0.42
1:N:578:LYS:NZ	1:O:222:ARG:HD3	2.35	0.42
1:C:401:GLN:HG3	1:C:436:TYR:CD1	2.55	0.42
1:A:283:THR:O	1:A:286:VAL:HG12	2.19	0.42
1:P:202:MSE:HE2	1:P:204:ASP:HA	2.01	0.42
1:B:359:THR:HG23	1:B:362:LYS:HD2	2.01	0.42
1:B:533:GLU:HG3	1:B:537:ASN:ND2	2.34	0.42
1:A:474:VAL:O	1:A:478:VAL:HG23	2.19	0.42
1:L:300:ASN:OD1	1:L:305:HIS:CE1	2.73	0.42
1:P:165:ARG:O	1:P:165:ARG:HD2	2.20	0.42
1:N:514:PRO:HA	1:N:515:PRO:HD3	1.96	0.42
1:C:433:LEU:HD13	1:C:433:LEU:C	2.40	0.42
1:A:394:ALA:HA	1:A:420:SER:HB3	2.00	0.42
1:L:356:ALA:O	1:L:358:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ASP:CA	1:E:202:MSE:HE1	2.49	0.42
1:G:553:ILE:O	1:G:557:VAL:HG23	2.18	0.42
1:J:59:LEU:HD13	1:J:64:GLN:CG	2.48	0.42
1:L:378:GLU:CA	1:L:403:ILE:HD11	2.48	0.42
1:I:389:LEU:CD1	1:I:407:MSE:HE3	2.48	0.42
1:K:325:MSE:HE2	1:K:492:LEU:HD22	2.01	0.42
1:J:381:VAL:CG1	1:J:407:MSE:HE1	2.49	0.42
1:H:580:LYS:O	1:H:580:LYS:HD3	2.19	0.42
1:M:374:MSE:CE	1:M:379:ASP:HB3	2.48	0.42
1:C:129:ARG:CG	1:D:91:ARG:HD3	2.49	0.42
1:K:166:ILE:HD12	1:K:179:ILE:HG13	2.00	0.42
1:K:375:LYS:HB2	1:K:375:LYS:HE3	1.62	0.42
1:J:575:GLU:CD	1:J:575:GLU:H	2.21	0.42
1:L:548:ASP:C	1:L:548:ASP:OD2	2.56	0.42
1:D:396:GLY:O	1:D:426:ALA:O	2.37	0.42
1:A:368:GLU:O	1:A:369:HIS:HB2	2.19	0.42
1:M:194:LYS:HA	1:M:195:PRO:HD3	1.91	0.42
1:D:505:GLU:O	1:D:509:GLU:HG3	2.19	0.42
1:J:157:ALA:HB2	1:J:479:ILE:HD11	2.00	0.42
1:N:551:ALA:O	1:N:554:ARG:HG2	2.19	0.42
1:K:416:ILE:HG13	1:K:433:LEU:CD2	2.38	0.42
1:O:24:LYS:HE3	1:O:47:GLN:O	2.20	0.42
1:L:354:ARG:HE	1:L:358:LEU:HD21	1.85	0.42
1:A:279:ASP:O	1:A:283:THR:CG2	2.66	0.42
1:C:359:THR:HG23	1:C:361:GLU:OE1	2.20	0.42
1:F:36:LYS:HD2	1:F:562:TYR:HB3	2.02	0.42
1:J:47:GLN:HE22	1:J:566:VAL:HG13	1.84	0.42
1:F:356:ALA:HB2	7:F:2051:HOH:O	2.18	0.42
1:G:91:ARG:HD3	1:H:129:ARG:CG	2.49	0.42
1:N:243:THR:HG21	1:N:273:TYR:CD2	2.53	0.42
1:D:300:ASN:OD1	1:D:305:HIS:HE1	2.03	0.42
1:H:342:TRP:CD2	1:H:367:HIS:HD2	2.38	0.42
1:C:358:LEU:HD12	1:C:358:LEU:HA	1.90	0.42
1:B:138:HIS:NE2	1:B:223:HIS:HE1	2.17	0.42
1:M:222:ARG:HH12	1:P:580:LYS:HD2	1.85	0.42
1:M:24:LYS:HD3	1:M:48:LEU:HD23	2.02	0.42
1:D:270:ARG:NH2	1:D:488:ASP:OD1	2.53	0.42
1:I:578:LYS:HZ3	1:L:222:ARG:HD3	1.85	0.42
1:N:474:VAL:O	1:N:478:VAL:HG23	2.18	0.42
1:D:467:ASN:HD21	3:D:1582:OXL:C2	2.32	0.42
1:P:296:ARG:HB2	1:P:507:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:MSE:HG3	1:P:544:PRO:CD	2.50	0.42
1:D:401:GLN:O	1:D:405:GLN:HG3	2.19	0.42
1:F:354:ARG:NH2	1:F:358:LEU:HD12	2.34	0.42
1:G:229:GLN:HA	1:G:229:GLN:NE2	2.35	0.42
1:A:154:VAL:O	1:A:154:VAL:HG13	2.20	0.42
1:D:288:VAL:O	1:D:292:LEU:HD13	2.19	0.42
1:O:194:LYS:HA	1:O:195:PRO:HD3	1.84	0.42
1:E:204:ASP:OD1	1:F:56:PRO:HG3	2.20	0.42
1:E:263:PHE:CZ	1:E:314:GLU:HA	2.55	0.42
1:N:137:ILE:HB	1:N:205:VAL:HG12	2.01	0.42
1:O:160:VAL:HG21	1:O:238:PHE:CZ	2.55	0.42
1:M:104:ILE:CG2	1:M:105:GLU:N	2.82	0.42
1:B:104:ILE:CG1	1:B:108:MSE:CE	2.96	0.42
1:I:146:MSE:HE2	1:J:52:GLY:HA3	2.02	0.42
1:B:323:ILE:O	1:B:327:MSE:HG3	2.20	0.42
1:H:184:LEU:HD12	1:H:200:PRO:HB3	2.01	0.42
1:M:548:ASP:OD2	1:M:551:ALA:CB	2.68	0.42
1:F:569:SER:HA	1:H:46:GLN:OE1	2.20	0.42
1:K:354:ARG:HG2	1:K:356:ALA:H	1.84	0.42
1:L:493:THR:O	1:L:497:VAL:HG23	2.20	0.42
1:E:224:LYS:CE	7:E:2029:HOH:O	2.68	0.42
1:P:160:VAL:CG1	1:P:161:THR:N	2.83	0.42
1:K:378:GLU:OE1	1:K:402:GLN:HB2	2.20	0.42
1:B:158:ILE:HG22	1:B:160:VAL:HG23	2.01	0.42
1:O:166:ILE:HD12	1:O:179:ILE:CG1	2.50	0.42
1:E:322:LEU:HD23	1:E:322:LEU:HA	1.78	0.42
1:F:61:GLN:NE2	1:F:98:LYS:HG2	2.34	0.42
1:C:270:ARG:NH1	1:C:270:ARG:CG	2.82	0.42
1:E:374:MSE:HE1	1:E:379:ASP:CB	2.49	0.42
1:C:467:ASN:O	1:C:470:VAL:N	2.40	0.42
1:H:166:ILE:HD12	1:H:179:ILE:HG13	2.01	0.42
1:L:399:PHE:CD2	1:L:427:GLU:HB3	2.54	0.42
1:K:454:LEU:HD12	1:K:454:LEU:N	2.35	0.42
1:L:301:ARG:NH2	7:L:2039:HOH:O	2.53	0.42
1:K:352:LYS:HG3	1:K:366:ALA:O	2.20	0.42
1:H:145:THR:O	1:H:148:GLN:HB2	2.20	0.42
1:H:148:GLN:HA	1:H:245:ARG:NH2	2.35	0.42
1:N:460:LEU:HA	1:N:509:GLU:O	2.20	0.42
1:F:548:ASP:OD2	1:F:551:ALA:HB2	2.19	0.42
1:D:502:VAL:HG22	1:D:514:PRO:HD3	2.02	0.42
1:A:433:LEU:CD1	1:A:443:PHE:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:386:PRO:HG2	1:H:407:MSE:CE	2.34	0.42
1:O:238:PHE:O	1:O:242:VAL:HG23	2.20	0.42
1:O:36:LYS:HD2	1:O:562:TYR:HB3	2.01	0.42
1:C:431:GLU:OE2	1:C:452:VAL:HG13	2.19	0.42
1:D:270:ARG:HH12	1:D:487:GLY:HA2	1.84	0.42
1:E:177:MSE:HE2	1:E:202:MSE:CB	2.50	0.42
1:B:429:THR:CG2	1:B:430:ALA:N	2.83	0.42
1:C:389:LEU:HG	1:C:407:MSE:HE3	2.01	0.42
1:M:502:VAL:HG12	1:M:507:LEU:HD13	2.00	0.42
1:K:207:THR:HA	1:K:225:ARG:HG2	2.02	0.42
1:B:401:GLN:O	1:B:405:GLN:HB2	2.20	0.42
1:D:150:TRP:HA	1:D:151:PRO:HD2	1.84	0.42
1:G:104:ILE:O	1:G:108:MSE:HB2	2.19	0.42
1:E:395:ILE:O	1:E:396:GLY:C	2.58	0.42
1:A:91:ARG:NH1	1:B:128:ARG:HA	2.34	0.42
1:M:248:MSE:HG3	1:P:544:PRO:HD2	2.01	0.42
1:P:222:ARG:NH1	1:P:222:ARG:HG3	2.34	0.42
1:E:467:ASN:ND2	3:E:1582:OXL:O2	2.53	0.42
1:C:349:LEU:HB2	1:C:380:ILE:CD1	2.50	0.42
1:C:259:ASN:HB3	7:C:2034:HOH:O	2.19	0.42
1:B:31:ASP:HA	1:B:32:PRO:HD2	1.90	0.42
1:N:59:LEU:HD12	1:N:59:LEU:O	2.19	0.42
1:G:378:GLU:O	1:G:382:LYS:HG3	2.20	0.42
1:M:435:LYS:HE3	1:M:436:TYR:CZ	2.55	0.42
1:L:394:ALA:HA	1:L:420:SER:HB3	2.02	0.42
1:O:428:CYS:CB	1:O:432:GLN:HE21	2.33	0.42
1:H:154:VAL:O	1:H:154:VAL:CG1	2.66	0.42
1:G:160:VAL:HG11	1:G:238:PHE:CZ	2.55	0.42
1:E:297:ILE:CG1	1:E:507:LEU:HD12	2.49	0.42
1:G:155:ILE:HD13	1:G:246:TYR:CZ	2.55	0.42
1:H:72:PHE:CZ	1:H:81:ARG:HD3	2.55	0.42
1:K:389:LEU:HD13	1:K:399:PHE:CZ	2.54	0.42
1:C:359:THR:CG2	1:C:361:GLU:H	2.33	0.42
1:I:328:GLN:HA	1:I:332:VAL:O	2.19	0.42
1:C:345:ASP:OD1	1:C:354:ARG:NH2	2.52	0.42
1:L:315:ALA:O	1:L:319:ILE:HG13	2.19	0.42
1:N:96:PHE:CZ	1:N:100:LEU:HD11	2.54	0.42
1:D:554:ARG:NH1	1:D:554:ARG:HG2	2.34	0.42
1:P:108:MSE:N	1:P:109:PRO:CD	2.83	0.42
1:M:512:LEU:HD23	1:M:512:LEU:HA	1.89	0.42
1:L:133:LEU:HA	1:L:133:LEU:HD23	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:LYS:HD2	1:L:27:GLU:HG2	2.00	0.42
1:A:160:VAL:HG13	1:A:201:VAL:HB	2.02	0.42
1:M:51:HIS:CD2	1:N:146:MSE:HE3	2.54	0.42
1:P:429:THR:CG2	1:P:431:GLU:H	2.26	0.41
1:B:250:CYS:O	1:B:252:ILE:HD12	2.20	0.41
1:O:23:LYS:HG3	1:O:24:LYS:N	2.34	0.41
1:J:401:GLN:HG2	1:J:436:TYR:CE2	2.54	0.41
1:F:113:THR:HG23	1:F:114:PRO:HA	2.01	0.41
1:N:225:ARG:HB2	1:N:227:ARG:NH1	2.35	0.41
1:C:317:LEU:HD23	1:C:343:MSE:HE1	2.01	0.41
1:C:261:ASN:OD1	1:C:264:ARG:NH1	2.50	0.41
1:K:108:MSE:HB3	1:K:109:PRO:HD3	2.02	0.41
1:F:514:PRO:HA	1:F:515:PRO:HD3	1.97	0.41
1:F:418:ALA:O	1:F:445:SER:HA	2.20	0.41
1:K:395:ILE:O	1:K:396:GLY:C	2.58	0.41
1:E:571:THR:OG1	1:E:577:MSE:SE	2.88	0.41
1:L:564:CYS:SG	1:L:566:VAL:HB	2.60	0.41
1:I:309:PHE:HE1	1:I:341:ILE:HG23	1.84	0.41
1:D:442:ILE:CG2	1:D:512:LEU:HD21	2.50	0.41
1:E:136:THR:CG2	1:E:137:ILE:N	2.83	0.41
1:C:497:VAL:HG11	1:C:526:ILE:HD13	2.02	0.41
1:L:104:ILE:HG23	1:L:105:GLU:N	2.35	0.41
1:L:165:ARG:HD2	1:L:165:ARG:C	2.40	0.41
1:M:108:MSE:N	1:M:109:PRO:CD	2.83	0.41
1:P:92:ASN:ND2	1:P:95:LEU:H	2.17	0.41
1:M:314:GLU:HB2	2:M:1581:NAP:O1N	2.19	0.41
1:L:322:LEU:HD23	1:L:322:LEU:HA	1.92	0.41
1:N:202:MSE:HE2	1:N:204:ASP:HB2	2.02	0.41
1:E:74:ARG:HD3	1:F:125:LEU:HD11	2.02	0.41
1:D:162:ASP:O	1:D:225:ARG:NH2	2.43	0.41
1:D:343:MSE:HB2	1:D:350:ILE:HD12	2.03	0.41
1:H:342:TRP:CZ3	1:H:367:HIS:HB2	2.55	0.41
1:I:264:ARG:NH1	1:I:264:ARG:HB3	2.35	0.41
1:O:504:GLU:HG3	1:O:508:GLN:NE2	2.35	0.41
1:J:215:ASP:HB3	1:J:218:TYR:HB2	2.01	0.41
1:J:158:ILE:HD12	1:J:242:VAL:HG11	2.02	0.41
1:P:141:GLY:H	1:P:237:GLU:CD	2.23	0.41
1:D:136:THR:HG22	1:D:139:ASP:OD1	2.20	0.41
1:E:327:MSE:HE1	1:E:337:ALA:O	2.20	0.41
1:E:160:VAL:HG11	1:E:238:PHE:CZ	2.55	0.41
1:L:297:ILE:HD11	1:L:507:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:ILE:CD1	1:I:507:LEU:HD12	2.49	0.41
1:H:274:CYS:SG	1:H:478:VAL:HG11	2.61	0.41
1:E:401:GLN:HG3	7:E:2038:HOH:O	2.20	0.41
1:B:172:LEU:O	1:B:175:TYR:HB2	2.19	0.41
1:J:243:THR:HG21	1:J:273:TYR:CD2	2.54	0.41
1:I:471:PHE:CG	1:I:472:PRO:HD3	2.56	0.41
1:B:215:ASP:OD1	1:B:216:PRO:HD2	2.20	0.41
1:C:118:LEU:HD11	5:C:1588:CL:CL	2.57	0.41
1:N:33:HIS:HD2	1:N:93:GLU:OE2	2.02	0.41
1:E:152:GLU:OE2	1:E:196:HIS:CE1	2.73	0.41
1:G:165:ARG:O	1:G:256:ASP:HB3	2.21	0.41
1:A:276:PHE:HB2	1:A:281:GLN:OE1	2.20	0.41
1:H:526:ILE:O	1:H:530:ILE:HG13	2.20	0.41
1:L:65:VAL:O	1:L:69:LEU:HG	2.21	0.41
1:F:209:ASN:OD1	1:F:211:THR:HB	2.20	0.41
1:O:476:LEU:HB3	1:O:527:ALA:HB2	2.01	0.41
1:M:574:GLU:HA	1:M:577:MSE:HE2	2.01	0.41
1:E:386:PRO:HG2	1:E:407:MSE:CE	2.28	0.41
1:P:323:ILE:HG22	1:P:327:MSE:HE2	2.02	0.41
1:J:429:THR:CG2	1:J:430:ALA:N	2.83	0.41
1:L:252:ILE:HD12	1:L:252:ILE:N	2.36	0.41
1:G:429:THR:HG23	1:G:449:PHE:CD2	2.55	0.41
1:F:68:ILE:HG13	1:F:95:LEU:HD11	2.01	0.41
1:H:402:GLN:HG3	7:H:2045:HOH:O	2.19	0.41
1:G:239:MSE:HE1	1:G:252:ILE:HG21	2.02	0.41
1:G:239:MSE:O	1:G:243:THR:OG1	2.39	0.41
1:D:92:ASN:ND2	1:D:92:ASN:C	2.64	0.41
1:G:242:VAL:HG13	1:G:246:TYR:CD1	2.53	0.41
1:B:322:LEU:HA	1:B:322:LEU:HD23	1.86	0.41
1:J:471:PHE:CG	1:J:472:PRO:HD3	2.55	0.41
1:H:194:LYS:HA	1:H:195:PRO:HD3	1.82	0.41
1:C:72:PHE:CE1	1:C:81:ARG:HB3	2.55	0.41
1:I:554:ARG:HG2	1:I:554:ARG:NH1	2.34	0.41
1:F:195:PRO:HD2	1:F:558:TYR:CE1	2.55	0.41
1:C:458:GLN:HB3	1:C:458:GLN:HE21	1.66	0.41
1:F:150:TRP:HA	1:F:151:PRO:HD2	1.84	0.41
1:K:254:PHE:CE2	1:K:265:LEU:HD13	2.56	0.41
1:M:141:GLY:H	1:M:237:GLU:CD	2.22	0.41
1:L:380:ILE:O	1:L:384:ILE:HG12	2.20	0.41
1:L:572:TRP:O	1:L:573:PRO:C	2.58	0.41
1:N:59:LEU:HD11	1:N:64:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:GLU:OE2	1:D:547:GLU:N	2.50	0.41
1:A:36:LYS:HE2	1:A:562:TYR:HB3	2.02	0.41
1:K:61:GLN:HA	1:K:64:GLN:HE21	1.85	0.41
1:D:433:LEU:CD1	1:D:443:PHE:HB2	2.51	0.41
1:F:401:GLN:CG	1:F:436:TYR:CZ	3.01	0.41
1:A:150:TRP:CD1	1:A:155:ILE:HD11	2.55	0.41
1:N:466:ASN:OD1	1:N:467:ASN:N	2.53	0.41
1:P:61:GLN:HE22	1:P:98:LYS:HE3	1.84	0.41
1:A:207:THR:HA	1:A:225:ARG:NH1	2.34	0.41
1:N:141:GLY:H	1:N:237:GLU:CD	2.21	0.41
1:F:467:ASN:HB3	1:F:471:PHE:HD2	1.84	0.41
1:B:207:THR:HA	1:B:225:ARG:HG2	2.02	0.41
1:F:194:LYS:HA	1:F:195:PRO:HD3	1.95	0.41
1:A:100:LEU:HD21	1:A:111:VAL:HG21	2.01	0.41
1:B:307:VAL:HG22	1:B:388:VAL:HB	2.02	0.41
1:P:292:LEU:HA	1:P:292:LEU:HD12	1.94	0.41
1:O:105:GLU:HB2	7:O:2024:HOH:O	2.19	0.41
1:M:90:ASP:OD1	1:M:131:ARG:NH1	2.53	0.41
1:K:274:CYS:SG	1:K:478:VAL:HG11	2.60	0.41
1:C:500:GLN:HB3	7:C:2063:HOH:O	2.19	0.41
1:F:158:ILE:HG12	1:F:199:LEU:HB3	2.01	0.41
1:P:184:LEU:HD22	1:P:198:CYS:HB3	2.01	0.41
1:N:420:SER:HA	2:N:1581:NAP:H1D	2.02	0.41
1:K:498:ILE:CD1	1:K:526:ILE:HD11	2.48	0.41
1:O:350:ILE:CD1	1:O:362:LYS:HD2	2.50	0.41
1:P:202:MSE:HE3	1:P:203:LEU:C	2.41	0.41
1:P:350:ILE:HD11	1:P:362:LYS:HD3	2.01	0.41
1:H:177:MSE:O	1:H:180:PRO:HD2	2.21	0.41
1:B:85:LEU:HD12	1:B:110:ILE:CG2	2.51	0.41
1:K:79:LEU:HD13	1:K:118:LEU:HD12	2.03	0.41
1:M:144:ALA:HB2	7:M:2022:HOH:O	2.20	0.41
1:B:212:LEU:HD13	1:B:218:TYR:CE1	2.55	0.41
1:A:243:THR:HG21	1:A:273:TYR:CD2	2.55	0.41
1:G:50:ILE:HA	1:G:53:LEU:HD12	2.02	0.41
1:P:332:VAL:CG2	1:P:336:GLU:HB3	2.51	0.41
1:L:429:THR:CG2	1:L:430:ALA:N	2.84	0.41
1:P:44:GLU:O	1:P:48:LEU:HB2	2.20	0.41
1:D:416:ILE:HG13	1:D:433:LEU:CD2	2.41	0.41
1:G:395:ILE:O	1:G:396:GLY:C	2.59	0.41
1:G:239:MSE:CE	1:G:254:PHE:CZ	3.02	0.41
1:G:389:LEU:HD22	1:G:399:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:140:ARG:HG2	1:N:234:LEU:HD13	2.03	0.41
1:N:265:LEU:HA	1:N:265:LEU:HD23	1.84	0.41
1:H:77:SER:O	1:H:81:ARG:HG3	2.21	0.41
1:L:284:ALA:HB1	1:L:322:LEU:HB2	2.02	0.41
1:M:86:MSE:CE	1:M:89:GLN:NE2	2.84	0.41
1:O:460:LEU:HA	1:O:509:GLU:O	2.20	0.41
1:D:174:CYS:HA	1:D:202:MSE:HE3	2.02	0.41
1:N:502:VAL:CG1	1:N:507:LEU:HD13	2.50	0.41
1:F:393:ALA:HB3	7:F:2057:HOH:O	2.20	0.41
1:B:24:LYS:HZ3	1:D:24:LYS:HD3	1.86	0.41
1:K:381:VAL:HG21	1:K:403:ILE:HD12	2.03	0.41
1:J:404:LEU:HD13	1:J:433:LEU:HA	2.02	0.41
1:N:140:ARG:HB3	1:N:140:ARG:CZ	2.50	0.41
1:C:194:LYS:HA	1:C:195:PRO:HD3	1.87	0.41
1:J:328:GLN:HA	1:J:332:VAL:O	2.21	0.41
1:B:350:ILE:HG12	1:B:354:ARG:NH2	2.35	0.41
1:I:266:LEU:O	1:I:270:ARG:HB2	2.21	0.41
1:O:151:PRO:HB3	1:P:26:TYR:CE2	2.55	0.41
1:I:121:GLN:NE2	1:I:169:LEU:HD13	2.36	0.41
1:E:232:ASP:OD1	1:E:264:ARG:NH2	2.54	0.41
1:E:394:ALA:HA	1:E:420:SER:HB3	2.03	0.41
1:C:120:CYS:O	1:C:175:TYR:HB3	2.21	0.41
1:G:30:ARG:HD3	1:H:30:ARG:O	2.20	0.41
1:I:58:PHE:CD1	1:I:58:PHE:N	2.89	0.41
1:O:245:ARG:CG	1:O:245:ARG:HH11	2.34	0.41
1:C:26:TYR:H	1:C:26:TYR:HD2	1.69	0.41
1:L:395:ILE:O	1:L:396:GLY:C	2.59	0.41
1:G:285:SER:HB3	1:G:470:VAL:HG21	2.03	0.41
1:A:51:HIS:NE2	1:B:139:ASP:OD2	2.44	0.41
1:K:136:THR:CG2	1:K:138:HIS:HB2	2.51	0.41
1:O:136:THR:HG22	1:O:137:ILE:N	2.35	0.41
1:P:143:ILE:CD1	1:P:237:GLU:HG2	2.40	0.41
1:F:177:MSE:CE	1:F:180:PRO:HG2	2.51	0.41
1:P:504:GLU:CG	1:P:508:GLN:HE22	2.15	0.41
1:D:23:LYS:CG	1:D:24:LYS:N	2.73	0.41
1:L:109:PRO:HA	1:L:113:THR:O	2.21	0.41
1:O:64:GLN:NE2	1:O:562:TYR:OH	2.51	0.41
1:J:359:THR:HG23	1:J:362:LYS:N	2.22	0.41
1:O:270:ARG:CG	1:O:270:ARG:NH1	2.84	0.41
1:D:154:VAL:C	1:D:155:ILE:HD12	2.41	0.41
1:C:127:PHE:CE2	1:D:38:MSE:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LEU:HB2	1:F:63:ALA:HB3	2.02	0.41
1:A:150:TRP:CE2	1:A:199:LEU:HD13	2.56	0.41
1:J:41:THR:CG2	1:J:42:LEU:N	2.83	0.41
1:M:270:ARG:NH2	1:M:488:ASP:OD1	2.54	0.41
1:E:207:THR:HA	1:E:225:ARG:HG2	2.03	0.41
1:H:466:ASN:HA	2:H:1581:NAP:N7N	2.33	0.41
1:B:399:PHE:CG	1:B:427:GLU:HB3	2.56	0.41
1:M:177:MSE:C	1:M:180:PRO:HD2	2.40	0.41
1:N:123:TYR:HB3	1:N:175:TYR:CD2	2.56	0.41
1:G:183:LYS:HZ2	1:G:467:ASN:HD22	1.68	0.41
1:O:467:ASN:H	2:O:1581:NAP:H72N	1.69	0.41
1:O:359:THR:HG22	1:O:362:LYS:CE	2.47	0.41
1:P:207:THR:HA	1:P:225:ARG:HG2	2.03	0.41
1:P:162:ASP:CA	1:P:202:MSE:HE1	2.50	0.41
1:K:156:LYS:NZ	1:K:197:GLN:NE2	2.69	0.41
1:F:192:GLY:CA	1:F:557:VAL:HG13	2.50	0.41
1:O:78:ASP:HA	1:O:81:ARG:HH11	1.86	0.41
1:F:190:CYS:HB3	1:F:519:ILE:HG12	2.02	0.41
1:K:29:LEU:HA	1:K:35:ASN:ND2	2.36	0.41
1:P:471:PHE:N	1:P:472:PRO:CD	2.84	0.41
1:N:184:LEU:O	1:N:187:TYR:HB2	2.21	0.41
1:E:394:ALA:HB2	2:E:1581:NAP:O3D	2.21	0.41
1:E:471:PHE:CG	1:E:472:PRO:HD3	2.55	0.41
1:C:350:ILE:HG23	1:C:358:LEU:HD11	2.01	0.41
1:K:343:MSE:HE3	1:K:350:ILE:HD12	2.02	0.41
1:E:172:LEU:O	1:E:175:TYR:HB2	2.21	0.41
1:D:194:LYS:HA	1:D:195:PRO:HD3	1.89	0.41
1:P:473:GLY:N	5:P:1590:CL:CL	2.84	0.41
1:B:266:LEU:O	1:B:270:ARG:HB2	2.21	0.41
1:J:143:ILE:HG13	1:J:237:GLU:OE2	2.21	0.41
1:K:243:THR:HG21	1:K:273:TYR:CD2	2.56	0.41
1:O:155:ILE:N	1:O:155:ILE:HD12	2.35	0.41
1:D:471:PHE:N	1:D:472:PRO:CD	2.84	0.41
1:H:89:GLN:HG3	1:H:96:PHE:CD2	2.55	0.41
1:E:52:GLY:O	1:F:133:LEU:HD23	2.21	0.41
1:D:72:PHE:CE1	1:D:81:ARG:HB3	2.56	0.41
1:E:110:ILE:O	1:E:115:THR:HB	2.20	0.41
1:P:342:TRP:CD2	1:P:367:HIS:HD2	2.39	0.41
1:P:160:VAL:HG21	1:P:238:PHE:CZ	2.56	0.41
1:E:443:PHE:CG	1:E:444:ALA:N	2.89	0.41
1:N:59:LEU:CD1	1:N:64:GLN:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:407:MSE:HG2	1:L:416:ILE:HD11	2.01	0.41
1:J:315:ALA:O	1:J:319:ILE:HG13	2.20	0.41
1:J:164:GLU:CG	1:J:258:ALA:HB2	2.48	0.41
1:F:23:LYS:N	1:F:24:LYS:NZ	2.64	0.41
1:B:104:ILE:CG2	1:B:105:GLU:N	2.83	0.41
1:A:59:LEU:HD13	1:A:64:GLN:CG	2.52	0.41
1:G:352:LYS:HZ1	1:G:366:ALA:HB3	1.86	0.41
1:B:303:SER:CB	1:B:332:VAL:HG21	2.51	0.41
1:N:202:MSE:HE3	1:N:204:ASP:N	2.36	0.41
1:F:109:PRO:HA	1:F:113:THR:O	2.20	0.41
1:B:125:LEU:HD13	1:B:125:LEU:C	2.41	0.41
1:B:154:VAL:C	1:B:155:ILE:HD12	2.41	0.41
1:G:119:ALA:O	1:G:123:TYR:N	2.54	0.41
1:N:471:PHE:CD1	1:N:472:PRO:HD3	2.56	0.41
1:N:551:ALA:HA	1:N:554:ARG:HD2	2.03	0.41
1:K:343:MSE:O	1:K:349:LEU:HD12	2.20	0.41
1:K:421:ASN:HB3	1:K:422:PRO:HA	2.03	0.41
1:P:374:MSE:HE1	1:P:379:ASP:C	2.41	0.41
1:E:194:LYS:HA	1:E:195:PRO:HD3	1.89	0.41
1:L:100:LEU:HD21	1:L:111:VAL:HG21	2.03	0.41
1:M:384:ILE:O	1:M:385:LYS:C	2.60	0.41
1:O:332:VAL:HG22	1:O:333:SER:N	2.36	0.40
1:P:133:LEU:HD22	1:P:135:ILE:CG1	2.46	0.40
1:F:429:THR:N	1:F:432:GLN:NE2	2.51	0.40
1:J:429:THR:HB	1:J:432:GLN:CG	2.39	0.40
1:O:416:ILE:HG13	1:O:433:LEU:CD2	2.48	0.40
1:N:431:GLU:OE2	1:N:452:VAL:HG22	2.21	0.40
1:D:61:GLN:NE2	1:D:560:THR:HG23	2.35	0.40
1:C:399:PHE:HB2	1:C:428:CYS:HB3	2.03	0.40
1:A:92:ASN:ND2	1:A:95:LEU:H	2.19	0.40
1:J:145:THR:O	1:J:148:GLN:HB2	2.20	0.40
1:G:59:LEU:HB2	1:G:63:ALA:HB3	2.03	0.40
1:C:467:ASN:ND2	3:C:1582:OXL:C2	2.84	0.40
1:J:177:MSE:CE	1:J:202:MSE:HB2	2.50	0.40
1:H:168:GLY:O	1:H:425:LYS:HE3	2.21	0.40
1:E:165:ARG:C	1:E:165:ARG:HD2	2.41	0.40
1:I:120:CYS:O	1:I:175:TYR:HB3	2.22	0.40
1:G:502:VAL:CG1	1:G:507:LEU:HD13	2.51	0.40
1:M:94:LYS:HB2	1:M:562:TYR:CE2	2.56	0.40
1:J:516:LEU:N	1:J:516:LEU:HD22	2.36	0.40
1:H:268:LYS:HG2	1:H:269:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:354:ARG:HB3	1:K:358:LEU:HD11	2.02	0.40
1:A:113:THR:CG2	1:A:114:PRO:HA	2.51	0.40
1:K:365:PHE:CD1	1:K:365:PHE:N	2.88	0.40
1:C:484:LYS:HB3	1:C:485:HIS:CD2	2.56	0.40
1:A:414:PRO:HG2	1:A:441:GLY:HA2	2.02	0.40
1:H:136:THR:HG22	1:H:137:ILE:N	2.36	0.40
1:P:135:ILE:HD13	1:P:143:ILE:HG23	2.03	0.40
1:L:108:MSE:HB3	1:L:109:PRO:HD3	2.03	0.40
1:M:109:PRO:HA	1:M:113:THR:O	2.22	0.40
1:F:59:LEU:HD13	1:F:64:GLN:CG	2.51	0.40
1:E:202:MSE:CE	1:E:203:LEU:O	2.70	0.40
1:K:270:ARG:NH2	1:K:488:ASP:OD1	2.53	0.40
1:J:502:VAL:CG1	1:J:507:LEU:HD22	2.46	0.40
1:C:186:LEU:HD22	1:C:190:CYS:SG	2.62	0.40
1:I:352:LYS:HD3	1:I:352:LYS:HA	1.84	0.40
1:P:131:ARG:HH11	1:P:131:ARG:HB2	1.84	0.40
1:P:350:ILE:HG23	1:P:358:LEU:HD11	2.02	0.40
1:N:413:ARG:HD3	7:N:2047:HOH:O	2.20	0.40
1:A:417:PHE:CE1	1:A:444:ALA:HB3	2.57	0.40
1:G:36:LYS:CD	1:G:562:TYR:HB3	2.51	0.40
1:C:152:GLU:OE1	1:C:196:HIS:CE1	2.75	0.40
1:E:84:LEU:HD23	1:E:84:LEU:C	2.41	0.40
1:P:26:TYR:N	1:P:26:TYR:CD2	2.89	0.40
1:I:223:HIS:C	1:I:223:HIS:CD2	2.94	0.40
1:J:88:LEU:O	1:J:88:LEU:HD23	2.20	0.40
1:A:235:LEU:HA	1:A:235:LEU:HD13	1.85	0.40
1:A:231:TYR:O	1:A:235:LEU:HD23	2.21	0.40
1:A:245:ARG:HG2	1:A:246:TYR:CE2	2.56	0.40
1:G:494:THR:HG23	1:G:526:ILE:HG23	2.03	0.40
1:D:212:LEU:HD13	1:D:218:TYR:CE1	2.56	0.40
1:L:471:PHE:CG	1:L:472:PRO:HD3	2.56	0.40
1:F:66:TYR:O	1:F:70:LYS:HG2	2.21	0.40
1:P:199:LEU:HG	1:P:201:VAL:HG23	2.03	0.40
1:P:404:LEU:HD22	1:P:433:LEU:HD23	2.03	0.40
1:N:416:ILE:HG21	1:N:433:LEU:HD23	2.03	0.40
1:N:433:LEU:HD13	1:N:433:LEU:C	2.41	0.40
1:M:401:GLN:HG3	1:M:436:TYR:CD1	2.56	0.40
1:K:270:ARG:HH12	1:K:487:GLY:HA2	1.85	0.40
1:P:154:VAL:O	1:P:154:VAL:CG1	2.66	0.40
1:M:59:LEU:HD13	1:M:64:GLN:CG	2.50	0.40
1:H:38:MSE:HB2	1:H:59:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:359:THR:HG22	1:O:362:LYS:HG3	2.03	0.40
1:O:354:ARG:HE	1:O:358:LEU:CD1	2.32	0.40
1:H:167:LEU:CD1	1:H:179:ILE:HD11	2.51	0.40
1:N:470:VAL:HG13	1:N:494:THR:HG21	2.03	0.40
1:G:466:ASN:HA	2:G:1581:NAP:H72N	1.87	0.40
1:N:112:TYR:CG	1:N:186:LEU:HD11	2.56	0.40
1:J:493:THR:HG23	1:J:529:ARG:NH1	2.36	0.40
1:L:281:GLN:HB3	1:L:491:PHE:CD1	2.56	0.40
1:B:128:ARG:HH11	1:B:128:ARG:HG2	1.86	0.40
1:N:69:LEU:HD22	1:N:106:ARG:NH1	2.36	0.40
1:J:575:GLU:OE2	1:J:575:GLU:N	2.37	0.40
1:F:215:ASP:HA	1:F:216:PRO:HD2	1.96	0.40
1:D:276:PHE:C	1:D:276:PHE:CD1	2.94	0.40
1:N:235:LEU:HA	1:N:235:LEU:HD13	1.90	0.40
1:F:383:ASP:C	1:F:383:ASP:OD1	2.59	0.40
1:E:157:ALA:HB2	1:E:479:ILE:HD11	2.04	0.40
1:G:503:SER:O	1:G:506:ASN:HB2	2.20	0.40
1:A:142:HIS:O	1:A:146:MSE:HG3	2.21	0.40
1:B:88:LEU:HD13	1:B:96:PHE:HA	2.02	0.40
1:C:110:ILE:O	1:C:115:THR:HB	2.22	0.40
1:O:413:ARG:HA	1:O:414:PRO:HD2	1.96	0.40
1:A:433:LEU:HD12	1:A:434:TYR:CE2	2.57	0.40
1:M:136:THR:CG2	1:M:138:HIS:HB2	2.51	0.40
1:F:177:MSE:CE	1:F:177:MSE:CA	2.96	0.40
1:L:158:ILE:HG22	1:L:160:VAL:HG23	2.04	0.40
1:L:132:GLY:HA3	1:L:177:MSE:HE3	2.02	0.40
1:O:429:THR:HG22	1:O:430:ALA:H	1.86	0.40
1:K:36:LYS:O	1:K:39:ALA:HB3	2.22	0.40
1:G:399:PHE:HB2	1:G:428:CYS:HB3	2.02	0.40
1:I:536:ARG:HD3	7:I:2069:HOH:O	2.21	0.40
1:D:564:CYS:SG	1:D:566:VAL:HG23	2.62	0.40
1:I:242:VAL:HG13	1:I:246:TYR:HD1	1.87	0.40
1:B:202:MSE:HE2	1:B:204:ASP:HA	2.04	0.40
1:N:72:PHE:CZ	1:N:81:ARG:HD3	2.56	0.40
1:D:467:ASN:O	1:D:470:VAL:N	2.40	0.40
1:H:507:LEU:HD12	1:H:511:ARG:O	2.21	0.40
1:K:209:ASN:HB3	1:K:212:LEU:HD12	2.04	0.40
1:P:165:ARG:HD2	1:P:165:ARG:C	2.41	0.40
1:H:44:GLU:O	1:H:48:LEU:HB2	2.22	0.40
1:E:226:ILE:HA	1:E:226:ILE:HD13	1.96	0.40
1:G:412:LYS:HB3	7:G:2042:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:ASP:HA	1:I:216:PRO:HD2	1.94	0.40
1:H:417:PHE:CD1	1:H:444:ALA:HB3	2.56	0.40
1:M:261:ASN:OD1	1:M:264:ARG:NH2	2.54	0.40
1:L:194:LYS:HA	1:L:195:PRO:HD3	1.84	0.40
1:H:259:ASN:HB3	7:H:2035:HOH:O	2.22	0.40
1:J:432:GLN:H	1:J:432:GLN:HG2	1.69	0.40
1:J:572:TRP:C	1:J:573:PRO:O	2.58	0.40
1:P:48:LEU:O	1:P:49:ASN:HB2	2.21	0.40
1:G:388:VAL:HG22	1:G:415:ILE:HD12	2.03	0.40
1:C:533:GLU:CD	1:C:536:ARG:HH11	2.25	0.40
1:I:108:MSE:CE	1:I:190:CYS:SG	3.08	0.40
1:P:162:ASP:OD1	1:P:162:ASP:C	2.60	0.40
1:D:166:ILE:HD12	1:D:179:ILE:CG1	2.51	0.40
1:L:157:ALA:HB2	1:L:479:ILE:HD11	2.04	0.40
1:N:194:LYS:HA	1:N:195:PRO:HD3	1.93	0.40
1:K:92:ASN:ND2	1:K:92:ASN:C	2.75	0.40
1:P:243:THR:HG21	1:P:273:TYR:HD2	1.86	0.40
1:G:174:CYS:HB2	1:G:220:GLY:HA3	2.04	0.40
1:O:316:ALA:HB1	1:O:343:MSE:HE2	2.02	0.40
1:N:184:LEU:HD12	1:N:200:PRO:HB3	2.04	0.40
1:A:303:SER:HB3	1:A:332:VAL:HG21	2.03	0.40
1:C:26:TYR:N	1:C:26:TYR:CD2	2.90	0.40
1:L:312:ALA:HA	1:L:316:ALA:HB3	2.03	0.40
1:N:395:ILE:O	1:N:396:GLY:C	2.60	0.40
1:G:514:PRO:HA	1:G:515:PRO:HD3	1.93	0.40
1:O:98:LYS:HD3	1:O:560:THR:HG21	2.04	0.40
1:C:505:GLU:HG3	7:C:2064:HOH:O	2.20	0.40
1:C:412:LYS:O	1:C:440:ARG:NH1	2.48	0.40
1:F:395:ILE:O	1:F:396:GLY:C	2.60	0.40
1:J:531:ALA:HB1	1:J:549:LEU:HD22	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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	553/555 (100%)	524 (95%)	23 (4%)	6 (1%)	17	31
1	B	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	39	61
1	C	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	39	61
1	D	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	39	61
1	E	553/555 (100%)	530 (96%)	22 (4%)	1 (0%)	52	75
1	F	553/555 (100%)	529 (96%)	22 (4%)	2 (0%)	39	61
1	G	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	34	55
1	H	553/555 (100%)	534 (97%)	16 (3%)	3 (0%)	34	55
1	I	553/555 (100%)	535 (97%)	17 (3%)	1 (0%)	52	75
1	J	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	34	55
1	K	553/555 (100%)	524 (95%)	27 (5%)	2 (0%)	39	61
1	L	553/555 (100%)	534 (97%)	14 (2%)	5 (1%)	21	37
1	M	553/555 (100%)	528 (96%)	23 (4%)	2 (0%)	39	61
1	N	553/555 (100%)	528 (96%)	21 (4%)	4 (1%)	26	46
1	O	553/555 (100%)	531 (96%)	18 (3%)	4 (1%)	26	46
1	P	553/555 (100%)	532 (96%)	18 (3%)	3 (0%)	34	55
All	All	8848/8880 (100%)	8481 (96%)	322 (4%)	45 (0%)	34	55

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLY
1	A	573	PRO
1	B	396	GLY
1	C	396	GLY
1	D	396	GLY
1	D	573	PRO
1	E	396	GLY
1	F	573	PRO
1	G	396	GLY
1	G	573	PRO
1	H	396	GLY
1	I	396	GLY
1	J	396	GLY
1	J	573	PRO

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Mol	Chain	Res	Type
1	K	396	GLY
1	L	396	GLY
1	M	396	GLY
1	N	352	LYS
1	N	396	GLY
1	N	573	PRO
1	O	396	GLY
1	P	396	GLY
1	P	573	PRO
1	B	468	SER
1	C	468	SER
1	F	396	GLY
1	H	468	SER
1	P	468	SER
1	A	259	ASN
1	A	468	SER
1	L	259	ASN
1	O	573	PRO
1	L	468	SER
1	A	25	GLY
1	G	392	VAL
1	J	392	VAL
1	L	392	VAL
1	O	392	VAL
1	H	392	VAL
1	K	392	VAL
1	N	392	VAL
1	A	392	VAL
1	L	56	PRO
1	M	56	PRO
1	O	56	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	467/453 (103%)	438 (94%)	29 (6%)	23	41
1	B	467/453 (103%)	438 (94%)	29 (6%)	23	41
1	C	467/453 (103%)	437 (94%)	30 (6%)	22	39
1	D	467/453 (103%)	439 (94%)	28 (6%)	24	43
1	E	467/453 (103%)	431 (92%)	36 (8%)	16	30
1	F	467/453 (103%)	434 (93%)	33 (7%)	18	34
1	G	467/453 (103%)	441 (94%)	26 (6%)	26	47
1	H	467/453 (103%)	437 (94%)	30 (6%)	22	39
1	I	467/453 (103%)	439 (94%)	28 (6%)	24	43
1	J	467/453 (103%)	437 (94%)	30 (6%)	22	39
1	K	467/453 (103%)	443 (95%)	24 (5%)	29	52
1	L	467/453 (103%)	437 (94%)	30 (6%)	22	39
1	M	467/453 (103%)	432 (92%)	35 (8%)	17	31
1	N	467/453 (103%)	443 (95%)	24 (5%)	29	52
1	O	467/453 (103%)	437 (94%)	30 (6%)	22	39
1	P	467/453 (103%)	430 (92%)	37 (8%)	15	28
All	All	7472/7248 (103%)	6993 (94%)	479 (6%)	22	39

All (479) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	57	CYS
1	A	59	LEU
1	A	77	SER
1	A	88	LEU
1	A	92	ASN
1	A	114	PRO
1	A	118	LEU
1	A	125	LEU
1	A	136	THR
1	A	160	VAL
1	A	187	TYR
1	A	196	HIS
1	A	251	LEU

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	347	LYS
1	A	359	THR
1	A	389	LEU
1	A	402	GLN
1	A	410	PHE
1	A	458	GLN
1	A	459	THR
1	A	476	LEU
1	A	500	GLN
1	A	507	LEU
1	A	533	GLU
1	A	556	GLN
1	A	573	PRO
1	A	575	GLU
1	B	27	GLU
1	B	43	GLU
1	B	57	CYS
1	B	59	LEU
1	B	73	GLU
1	B	88	LEU
1	B	92	ASN
1	B	100	LEU
1	B	105	GLU
1	B	113	THR
1	B	125	LEU
1	B	133	LEU
1	B	165	ARG
1	B	187	TYR
1	B	239	MSE
1	B	251	LEU
1	B	292	LEU
1	B	301	ARG
1	B	310	GLN
1	B	322	LEU
1	B	352	LYS
1	B	389	LEU
1	B	401	GLN
1	B	405	GLN
1	B	458	GLN
1	B	476	LEU
1	B	556	GLN

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Mol	Chain	Res	Type
1	B	560	THR
1	B	569	SER
1	C	41	THR
1	C	59	LEU
1	C	88	LEU
1	C	92	ASN
1	C	98	LYS
1	C	118	LEU
1	C	155	ILE
1	C	177	MSE
1	C	196	HIS
1	C	202	MSE
1	C	292	LEU
1	C	322	LEU
1	C	329	LYS
1	C	359	THR
1	C	364	HIS
1	C	378	GLU
1	C	389	LEU
1	C	410	PHE
1	C	438	GLU
1	C	476	LEU
1	C	500	GLN
1	C	507	LEU
1	C	516	LEU
1	C	521	GLN
1	C	556	GLN
1	C	560	THR
1	C	573	PRO
1	C	574	GLU
1	C	575	GLU
1	C	580	LYS
1	D	30	ARG
1	D	59	LEU
1	D	87	SER
1	D	88	LEU
1	D	92	ASN
1	D	133	LEU
1	D	136	THR
1	D	139	ASP
1	D	140	ARG
1	D	196	HIS

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Mol	Chain	Res	Type
1	D	240	GLU
1	D	251	LEU
1	D	259	ASN
1	D	322	LEU
1	D	364	HIS
1	D	378	GLU
1	D	389	LEU
1	D	410	PHE
1	D	454	LEU
1	D	476	LEU
1	D	500	GLN
1	D	516	LEU
1	D	521	GLN
1	D	533	GLU
1	D	547	GLU
1	D	556	GLN
1	D	560	THR
1	D	575	GLU
1	E	24	LYS
1	E	27	GLU
1	E	43	GLU
1	E	48	LEU
1	E	57	CYS
1	E	59	LEU
1	E	88	LEU
1	E	92	ASN
1	E	100	LEU
1	E	118	LEU
1	E	125	LEU
1	E	131	ARG
1	E	133	LEU
1	E	187	TYR
1	E	196	HIS
1	E	240	GLU
1	E	245	ARG
1	E	251	LEU
1	E	310	GLN
1	E	322	LEU
1	E	333	SER
1	E	340	ARG
1	E	360	PRO
1	E	364	HIS

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Mol	Chain	Res	Type
1	E	368	GLU
1	E	389	LEU
1	E	410	PHE
1	E	435	LYS
1	E	476	LEU
1	E	489	ASP
1	E	492	LEU
1	E	500	GLN
1	E	516	LEU
1	E	560	THR
1	E	573	PRO
1	E	575	GLU
1	F	24	LYS
1	F	30	ARG
1	F	57	CYS
1	F	59	LEU
1	F	88	LEU
1	F	92	ASN
1	F	129	ARG
1	F	133	LEU
1	F	140	ARG
1	F	152	GLU
1	F	177	MSE
1	F	196	HIS
1	F	227	ARG
1	F	244	SER
1	F	251	LEU
1	F	259	ASN
1	F	264	ARG
1	F	292	LEU
1	F	299	LYS
1	F	310	GLN
1	F	322	LEU
1	F	335	GLU
1	F	379	ASP
1	F	389	LEU
1	F	458	GLN
1	F	476	LEU
1	F	516	LEU
1	F	521	GLN
1	F	533	GLU
1	F	556	GLN

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Mol	Chain	Res	Type
1	F	560	THR
1	F	573	PRO
1	F	575	GLU
1	G	48	LEU
1	G	57	CYS
1	G	59	LEU
1	G	88	LEU
1	G	92	ASN
1	G	114	PRO
1	G	125	LEU
1	G	133	LEU
1	G	160	VAL
1	G	196	HIS
1	G	227	ARG
1	G	243	THR
1	G	292	LEU
1	G	322	LEU
1	G	335	GLU
1	G	352	LYS
1	G	363	GLU
1	G	389	LEU
1	G	410	PHE
1	G	412	LYS
1	G	476	LEU
1	G	500	GLN
1	G	507	LEU
1	G	556	GLN
1	G	575	GLU
1	G	580	LYS
1	H	27	GLU
1	H	47	GLN
1	H	48	LEU
1	H	57	CYS
1	H	59	LEU
1	H	62	ASP
1	H	88	LEU
1	H	92	ASN
1	H	111	VAL
1	H	133	LEU
1	H	140	ARG
1	H	165	ARG
1	H	196	HIS

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Mol	Chain	Res	Type
1	H	223	HIS
1	H	251	LEU
1	H	322	LEU
1	H	358	LEU
1	H	359	THR
1	H	389	LEU
1	H	476	LEU
1	H	500	GLN
1	H	505	GLU
1	H	507	LEU
1	H	516	LEU
1	H	539	THR
1	H	547	GLU
1	H	556	GLN
1	H	560	THR
1	H	575	GLU
1	H	578	LYS
1	I	48	LEU
1	I	49	ASN
1	I	59	LEU
1	I	61	GLN
1	I	73	GLU
1	I	88	LEU
1	I	92	ASN
1	I	131	ARG
1	I	133	LEU
1	I	165	ARG
1	I	187	TYR
1	I	223	HIS
1	I	285	SER
1	I	322	LEU
1	I	335	GLU
1	I	340	ARG
1	I	360	PRO
1	I	389	LEU
1	I	410	PHE
1	I	454	LEU
1	I	467	ASN
1	I	476	LEU
1	I	516	LEU
1	I	556	GLN
1	I	560	THR

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Mol	Chain	Res	Type
1	I	569	SER
1	I	575	GLU
1	I	578	LYS
1	J	27	GLU
1	J	59	LEU
1	J	67	SER
1	J	88	LEU
1	J	92	ASN
1	J	116	VAL
1	J	133	LEU
1	J	136	THR
1	J	140	ARG
1	J	165	ARG
1	J	187	TYR
1	J	202	MSE
1	J	251	LEU
1	J	292	LEU
1	J	322	LEU
1	J	363	GLU
1	J	389	LEU
1	J	405	GLN
1	J	476	LEU
1	J	489	ASP
1	J	500	GLN
1	J	504	GLU
1	J	505	GLU
1	J	507	LEU
1	J	521	GLN
1	J	533	GLU
1	J	538	ASN
1	J	556	GLN
1	J	560	THR
1	J	573	PRO
1	K	27	GLU
1	K	49	ASN
1	K	59	LEU
1	K	62	ASP
1	K	88	LEU
1	K	92	ASN
1	K	136	THR
1	K	139	ASP
1	K	165	ARG

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Mol	Chain	Res	Type
1	K	251	LEU
1	K	292	LEU
1	K	310	GLN
1	K	322	LEU
1	K	364	HIS
1	K	389	LEU
1	K	410	PHE
1	K	456	SER
1	K	476	LEU
1	K	489	ASP
1	K	533	GLU
1	K	556	GLN
1	K	560	THR
1	K	569	SER
1	K	578	LYS
1	L	48	LEU
1	L	57	CYS
1	L	59	LEU
1	L	88	LEU
1	L	92	ASN
1	L	152	GLU
1	L	177	MSE
1	L	187	TYR
1	L	196	HIS
1	L	224	LYS
1	L	239	MSE
1	L	245	ARG
1	L	251	LEU
1	L	261	ASN
1	L	310	GLN
1	L	321	ASN
1	L	322	LEU
1	L	352	LYS
1	L	364	HIS
1	L	389	LEU
1	L	456	SER
1	L	476	LEU
1	L	500	GLN
1	L	507	LEU
1	L	539	THR
1	L	547	GLU
1	L	556	GLN

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Mol	Chain	Res	Type
1	L	557	VAL
1	L	575	GLU
1	L	580	LYS
1	M	24	LYS
1	M	27	GLU
1	M	57	CYS
1	M	59	LEU
1	M	88	LEU
1	M	92	ASN
1	M	105	GLU
1	M	125	LEU
1	M	133	LEU
1	M	136	THR
1	M	165	ARG
1	M	196	HIS
1	M	251	LEU
1	M	292	LEU
1	M	310	GLN
1	M	322	LEU
1	M	332	VAL
1	M	336	GLU
1	M	352	LYS
1	M	358	LEU
1	M	360	PRO
1	M	364	HIS
1	M	389	LEU
1	M	433	LEU
1	M	450	ASP
1	M	467	ASN
1	M	476	LEU
1	M	505	GLU
1	M	507	LEU
1	M	538	ASN
1	M	556	GLN
1	M	560	THR
1	M	571	THR
1	M	575	GLU
1	M	578	LYS
1	N	24	LYS
1	N	77	SER
1	N	88	LEU
1	N	92	ASN

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Mol	Chain	Res	Type
1	N	105	GLU
1	N	125	LEU
1	N	133	LEU
1	N	139	ASP
1	N	152	GLU
1	N	187	TYR
1	N	196	HIS
1	N	310	GLN
1	N	321	ASN
1	N	322	LEU
1	N	389	LEU
1	N	410	PHE
1	N	456	SER
1	N	476	LEU
1	N	489	ASP
1	N	507	LEU
1	N	556	GLN
1	N	560	THR
1	N	573	PRO
1	N	578	LYS
1	O	57	CYS
1	O	59	LEU
1	O	88	LEU
1	O	92	ASN
1	O	133	LEU
1	O	165	ARG
1	O	177	MSE
1	O	187	TYR
1	O	196	HIS
1	O	232	ASP
1	O	245	ARG
1	O	251	LEU
1	O	302	LEU
1	O	303	SER
1	O	322	LEU
1	O	335	GLU
1	O	389	LEU
1	O	410	PHE
1	O	467	ASN
1	O	476	LEU
1	O	489	ASP
1	O	507	LEU

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Mol	Chain	Res	Type
1	O	516	LEU
1	O	521	GLN
1	O	533	GLU
1	O	547	GLU
1	O	556	GLN
1	O	560	THR
1	O	571	THR
1	O	575	GLU
1	P	48	LEU
1	P	57	CYS
1	P	58	PHE
1	P	59	LEU
1	P	62	ASP
1	P	73	GLU
1	P	88	LEU
1	P	92	ASN
1	P	113	THR
1	P	118	LEU
1	P	131	ARG
1	P	140	ARG
1	P	152	GLU
1	P	153	SER
1	P	155	ILE
1	P	183	LYS
1	P	196	HIS
1	P	251	LEU
1	P	264	ARG
1	P	292	LEU
1	P	310	GLN
1	P	322	LEU
1	P	385	LYS
1	P	389	LEU
1	P	410	PHE
1	P	438	GLU
1	P	454	LEU
1	P	476	LEU
1	P	500	GLN
1	P	507	LEU
1	P	508	GLN
1	P	516	LEU
1	P	521	GLN
1	P	533	GLU

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Mol	Chain	Res	Type
1	P	556	GLN
1	P	560	THR
1	P	573	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (286) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	35	ASN
1	A	61	GLN
1	A	64	GLN
1	A	89	GLN
1	A	92	ASN
1	A	122	HIS
1	A	223	HIS
1	A	229	GLN
1	A	305	HIS
1	A	310	GLN
1	A	328	GLN
1	A	432	GLN
1	A	508	GLN
1	A	545	GLN
1	A	556	GLN
1	B	33	HIS
1	B	35	ASN
1	B	61	GLN
1	B	64	GLN
1	B	89	GLN
1	B	92	ASN
1	B	223	HIS
1	B	305	HIS
1	B	328	GLN
1	B	364	HIS
1	B	401	GLN
1	B	402	GLN
1	B	432	GLN
1	B	458	GLN
1	B	508	GLN
1	B	521	GLN
1	B	537	ASN
1	B	545	GLN
1	B	556	GLN

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Mol	Chain	Res	Type
1	C	35	ASN
1	C	46	GLN
1	C	61	GLN
1	C	64	GLN
1	C	89	GLN
1	C	92	ASN
1	C	197	GLN
1	C	223	HIS
1	C	229	GLN
1	C	305	HIS
1	C	328	GLN
1	C	401	GLN
1	C	402	GLN
1	C	458	GLN
1	C	508	GLN
1	C	537	ASN
1	C	545	GLN
1	C	556	GLN
1	D	33	HIS
1	D	35	ASN
1	D	61	GLN
1	D	64	GLN
1	D	89	GLN
1	D	92	ASN
1	D	196	HIS
1	D	229	GLN
1	D	259	ASN
1	D	305	HIS
1	D	328	GLN
1	D	401	GLN
1	D	432	GLN
1	D	458	GLN
1	D	467	ASN
1	D	508	GLN
1	D	521	GLN
1	D	545	GLN
1	D	556	GLN
1	D	563	ASN
1	E	35	ASN
1	E	46	GLN
1	E	49	ASN
1	E	61	GLN

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Mol	Chain	Res	Type
1	E	64	GLN
1	E	92	ASN
1	E	122	HIS
1	E	223	HIS
1	E	305	HIS
1	E	328	GLN
1	E	500	GLN
1	E	538	ASN
1	E	545	GLN
1	F	33	HIS
1	F	35	ASN
1	F	61	GLN
1	F	64	GLN
1	F	89	GLN
1	F	92	ASN
1	F	197	GLN
1	F	223	HIS
1	F	259	ASN
1	F	267	HIS
1	F	305	HIS
1	F	328	GLN
1	F	432	GLN
1	F	458	GLN
1	F	467	ASN
1	F	521	GLN
1	F	545	GLN
1	F	556	GLN
1	G	33	HIS
1	G	35	ASN
1	G	51	HIS
1	G	61	GLN
1	G	64	GLN
1	G	89	GLN
1	G	92	ASN
1	G	122	HIS
1	G	148	GLN
1	G	223	HIS
1	G	229	GLN
1	G	305	HIS
1	G	328	GLN
1	G	401	GLN
1	G	432	GLN

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Mol	Chain	Res	Type
1	G	467	ASN
1	G	521	GLN
1	G	545	GLN
1	G	556	GLN
1	H	33	HIS
1	H	35	ASN
1	H	49	ASN
1	H	61	GLN
1	H	64	GLN
1	H	89	GLN
1	H	92	ASN
1	H	148	GLN
1	H	223	HIS
1	H	229	GLN
1	H	271	ASN
1	H	305	HIS
1	H	321	ASN
1	H	328	GLN
1	H	367	HIS
1	H	376	ASN
1	H	401	GLN
1	H	405	GLN
1	H	432	GLN
1	H	508	GLN
1	H	521	GLN
1	H	537	ASN
1	H	545	GLN
1	H	556	GLN
1	I	33	HIS
1	I	35	ASN
1	I	61	GLN
1	I	64	GLN
1	I	89	GLN
1	I	92	ASN
1	I	121	GLN
1	I	122	HIS
1	I	229	GLN
1	I	305	HIS
1	I	328	GLN
1	I	405	GLN
1	I	458	GLN
1	I	467	ASN

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Mol	Chain	Res	Type
1	I	537	ASN
1	I	545	GLN
1	I	556	GLN
1	J	33	HIS
1	J	35	ASN
1	J	49	ASN
1	J	61	GLN
1	J	64	GLN
1	J	89	GLN
1	J	92	ASN
1	J	122	HIS
1	J	223	HIS
1	J	259	ASN
1	J	305	HIS
1	J	328	GLN
1	J	364	HIS
1	J	432	GLN
1	J	467	ASN
1	J	545	GLN
1	J	556	GLN
1	J	563	ASN
1	K	33	HIS
1	K	35	ASN
1	K	46	GLN
1	K	61	GLN
1	K	64	GLN
1	K	89	GLN
1	K	92	ASN
1	K	148	GLN
1	K	197	GLN
1	K	259	ASN
1	K	305	HIS
1	K	310	GLN
1	K	401	GLN
1	K	402	GLN
1	K	432	GLN
1	K	467	ASN
1	K	508	GLN
1	K	545	GLN
1	K	556	GLN
1	L	35	ASN
1	L	49	ASN

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Mol	Chain	Res	Type
1	L	51	HIS
1	L	61	GLN
1	L	64	GLN
1	L	89	GLN
1	L	92	ASN
1	L	148	GLN
1	L	223	HIS
1	L	261	ASN
1	L	305	HIS
1	L	310	GLN
1	L	321	ASN
1	L	328	GLN
1	L	432	GLN
1	L	467	ASN
1	L	500	GLN
1	L	537	ASN
1	L	556	GLN
1	M	33	HIS
1	M	35	ASN
1	M	51	HIS
1	M	61	GLN
1	M	64	GLN
1	M	89	GLN
1	M	92	ASN
1	M	223	HIS
1	M	305	HIS
1	M	401	GLN
1	M	405	GLN
1	M	432	GLN
1	M	467	ASN
1	M	508	GLN
1	M	545	GLN
1	M	556	GLN
1	N	33	HIS
1	N	35	ASN
1	N	61	GLN
1	N	64	GLN
1	N	89	GLN
1	N	92	ASN
1	N	223	HIS
1	N	259	ASN
1	N	305	HIS

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Mol	Chain	Res	Type
1	N	328	GLN
1	N	458	GLN
1	N	464	GLN
1	N	467	ASN
1	N	508	GLN
1	N	545	GLN
1	N	556	GLN
1	O	33	HIS
1	O	35	ASN
1	O	61	GLN
1	O	64	GLN
1	O	89	GLN
1	O	92	ASN
1	O	223	HIS
1	O	267	HIS
1	O	305	HIS
1	O	328	GLN
1	O	401	GLN
1	O	402	GLN
1	O	405	GLN
1	O	432	GLN
1	O	467	ASN
1	O	508	GLN
1	O	537	ASN
1	O	545	GLN
1	O	556	GLN
1	P	33	HIS
1	P	35	ASN
1	P	61	GLN
1	P	64	GLN
1	P	89	GLN
1	P	92	ASN
1	P	223	HIS
1	P	229	GLN
1	P	305	HIS
1	P	402	GLN
1	P	432	GLN
1	P	500	GLN
1	P	508	GLN
1	P	545	GLN
1	P	556	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 117 ligands modelled in this entry, 85 are monoatomic - leaving 32 for Mogul analysis.

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$
2	NAP	A	1581	-	42,52,52	1.73	9 (21%)	54,80,80	2.10	5 (9%)
3	OXL	A	1583	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	B	1581	-	42,52,52	1.60	8 (19%)	54,80,80	2.04	8 (14%)
3	OXL	B	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	C	1581	-	42,52,52	1.68	6 (14%)	54,80,80	2.07	7 (12%)
3	OXL	C	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	D	1581	-	42,52,52	1.60	8 (19%)	54,80,80	2.16	7 (12%)
3	OXL	D	1582	4,6	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	E	1581	-	42,52,52	1.71	8 (19%)	54,80,80	2.11	6 (11%)
3	OXL	E	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	F	1581	-	42,52,52	1.58	7 (16%)	54,80,80	2.11	8 (14%)
3	OXL	F	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	G	1581	-	42,52,52	1.63	6 (14%)	54,80,80	2.10	6 (11%)
3	OXL	G	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	H	1581	-	42,52,52	1.68	8 (19%)	54,80,80	2.13	7 (12%)
3	OXL	H	1582	4	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	I	1581	-	42,52,52	1.75	11 (26%)	54,80,80	2.12	8 (14%)
3	OXL	I	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	J	1581	-	42,52,52	1.66	8 (19%)	54,80,80	2.15	8 (14%)
3	OXL	J	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	K	1581	-	42,52,52	1.75	8 (19%)	54,80,80	2.12	7 (12%)
3	OXL	K	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	L	1581	-	42,52,52	1.79	10 (23%)	54,80,80	2.10	6 (11%)
3	OXL	L	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	M	1581	-	42,52,52	1.59	8 (19%)	54,80,80	2.05	7 (12%)
3	OXL	M	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	N	1581	-	42,52,52	1.74	8 (19%)	54,80,80	2.12	8 (14%)
3	OXL	N	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	O	1581	-	42,52,52	1.68	9 (21%)	54,80,80	2.13	7 (12%)
3	OXL	O	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	P	1581	-	42,52,52	1.55	8 (19%)	54,80,80	2.08	7 (12%)
3	OXL	P	1582	4	0,5,5	0.00	-	0,6,6	0.00	-

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
2	NAP	A	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	A	1583	4	-	0/0/4/4	0/0/0/0
2	NAP	B	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	B	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	C	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	C	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	D	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	D	1582	4,6	-	0/0/4/4	0/0/0/0
2	NAP	E	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	E	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	F	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	F	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	G	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	G	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	H	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	H	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	I	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	I	1582	4	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	J	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	J	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	K	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	K	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	L	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	L	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	M	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	M	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	N	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	N	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	O	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	O	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	P	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	P	1582	4	-	0/0/4/4	0/0/0/0

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1581	NAP	C5A-C4A	-3.46	1.32	1.40
2	J	1581	NAP	C5A-C4A	-3.34	1.33	1.40
2	P	1581	NAP	C5A-C4A	-3.31	1.33	1.40
2	F	1581	NAP	C5A-C4A	-3.30	1.33	1.40
2	L	1581	NAP	C5A-C4A	-3.22	1.33	1.40
2	G	1581	NAP	C5A-C4A	-3.18	1.33	1.40
2	I	1581	NAP	C5A-C4A	-3.11	1.33	1.40
2	H	1581	NAP	C5A-C4A	-3.11	1.33	1.40
2	K	1581	NAP	C5A-C4A	-3.05	1.33	1.40
2	A	1581	NAP	C5A-C4A	-3.04	1.33	1.40
2	C	1581	NAP	C5A-C4A	-3.02	1.33	1.40
2	B	1581	NAP	C5A-C4A	-3.01	1.33	1.40
2	E	1581	NAP	C5A-C4A	-3.00	1.33	1.40
2	O	1581	NAP	C5A-C4A	-2.99	1.33	1.40
2	N	1581	NAP	C5A-C4A	-2.95	1.33	1.40
2	M	1581	NAP	C5A-C4A	-2.79	1.34	1.40
2	P	1581	NAP	C5A-N7A	-2.47	1.31	1.39
2	E	1581	NAP	C5A-N7A	-2.40	1.31	1.39
2	M	1581	NAP	C5A-N7A	-2.39	1.31	1.39
2	D	1581	NAP	C5A-N7A	-2.35	1.31	1.39
2	L	1581	NAP	C5A-N7A	-2.34	1.31	1.39
2	O	1581	NAP	C3B-C2B	-2.34	1.47	1.53
2	O	1581	NAP	C5A-N7A	-2.33	1.31	1.39
2	A	1581	NAP	C5A-N7A	-2.30	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1581	NAP	C5A-N7A	-2.25	1.31	1.39
2	N	1581	NAP	C5A-N7A	-2.23	1.31	1.39
2	J	1581	NAP	C5A-N7A	-2.20	1.32	1.39
2	H	1581	NAP	C5A-N7A	-2.19	1.32	1.39
2	I	1581	NAP	C5A-N7A	-2.12	1.32	1.39
2	B	1581	NAP	C5A-N7A	-2.10	1.32	1.39
2	F	1581	NAP	C5A-N7A	-2.02	1.32	1.39
2	I	1581	NAP	O4D-C4D	2.02	1.49	1.45
2	I	1581	NAP	C5N-C4N	2.03	1.43	1.38
2	N	1581	NAP	C2A-N1A	2.06	1.37	1.33
2	A	1581	NAP	C2A-N1A	2.08	1.37	1.33
2	P	1581	NAP	C5N-C4N	2.09	1.43	1.38
2	L	1581	NAP	C5N-C4N	2.10	1.43	1.38
2	B	1581	NAP	C2A-N1A	2.10	1.37	1.33
2	L	1581	NAP	C4N-C3N	2.14	1.42	1.39
2	O	1581	NAP	O4D-C4D	2.15	1.50	1.45
2	J	1581	NAP	C2A-N1A	2.15	1.38	1.33
2	I	1581	NAP	C2A-N1A	2.18	1.38	1.33
2	A	1581	NAP	C4N-C3N	2.20	1.43	1.39
2	D	1581	NAP	C2A-N1A	2.21	1.38	1.33
2	K	1581	NAP	C4N-C3N	2.25	1.43	1.39
2	H	1581	NAP	O4D-C4D	2.28	1.50	1.45
2	G	1581	NAP	C3N-C7N	2.30	1.54	1.50
2	M	1581	NAP	C2A-N1A	2.30	1.38	1.33
2	L	1581	NAP	C2A-N1A	2.31	1.38	1.33
2	E	1581	NAP	C2A-N1A	2.34	1.38	1.33
2	I	1581	NAP	C4N-C3N	2.40	1.43	1.39
2	O	1581	NAP	C3N-C7N	2.41	1.54	1.50
2	N	1581	NAP	C3N-C7N	2.45	1.54	1.50
2	P	1581	NAP	C3N-C7N	2.55	1.54	1.50
2	H	1581	NAP	C3N-C7N	2.56	1.54	1.50
2	J	1581	NAP	C3N-C7N	2.58	1.54	1.50
2	D	1581	NAP	C3N-C7N	2.67	1.54	1.50
2	F	1581	NAP	O4D-C1D	2.67	1.44	1.41
2	P	1581	NAP	O4D-C1D	2.71	1.44	1.41
2	M	1581	NAP	C3N-C7N	2.73	1.54	1.50
2	B	1581	NAP	C3N-C7N	2.77	1.54	1.50
2	M	1581	NAP	C2A-N3A	2.78	1.37	1.32
2	O	1581	NAP	C6N-N1N	2.79	1.43	1.35
2	B	1581	NAP	O4D-C1D	2.80	1.44	1.41
2	I	1581	NAP	C2A-N3A	2.82	1.37	1.32
2	O	1581	NAP	C2A-N3A	2.83	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1581	NAP	O4D-C1D	2.83	1.44	1.41
2	C	1581	NAP	C2A-N3A	2.85	1.37	1.32
2	F	1581	NAP	C2A-N3A	2.87	1.37	1.32
2	D	1581	NAP	C2A-N3A	2.89	1.37	1.32
2	J	1581	NAP	C2A-N3A	2.91	1.37	1.32
2	K	1581	NAP	C2A-N3A	2.99	1.37	1.32
2	A	1581	NAP	C2A-N3A	3.02	1.37	1.32
2	G	1581	NAP	C2A-N3A	3.03	1.37	1.32
2	D	1581	NAP	C6N-N1N	3.04	1.43	1.35
2	C	1581	NAP	C6N-N1N	3.07	1.43	1.35
2	P	1581	NAP	C2A-N3A	3.11	1.37	1.32
2	H	1581	NAP	C6N-N1N	3.13	1.43	1.35
2	L	1581	NAP	C2A-N3A	3.15	1.37	1.32
2	F	1581	NAP	C3N-C7N	3.16	1.55	1.50
2	A	1581	NAP	C3N-C7N	3.18	1.55	1.50
2	M	1581	NAP	C6N-N1N	3.25	1.44	1.35
2	G	1581	NAP	C6N-N1N	3.30	1.44	1.35
2	B	1581	NAP	C2A-N3A	3.31	1.38	1.32
2	E	1581	NAP	C6N-N1N	3.31	1.44	1.35
2	E	1581	NAP	C2A-N3A	3.31	1.38	1.32
2	O	1581	NAP	O4B-C1B	3.32	1.45	1.41
2	J	1581	NAP	O4B-C1B	3.34	1.45	1.41
2	J	1581	NAP	C6N-N1N	3.34	1.44	1.35
2	H	1581	NAP	C2A-N3A	3.36	1.38	1.32
2	B	1581	NAP	C6N-N1N	3.39	1.44	1.35
2	L	1581	NAP	C6N-N1N	3.40	1.44	1.35
2	F	1581	NAP	O4B-C1B	3.41	1.45	1.41
2	P	1581	NAP	O4B-C1B	3.42	1.45	1.41
2	L	1581	NAP	O4D-C1D	3.45	1.45	1.41
2	P	1581	NAP	C6N-N1N	3.47	1.44	1.35
2	A	1581	NAP	C6N-N1N	3.47	1.44	1.35
2	K	1581	NAP	C6N-N1N	3.48	1.44	1.35
2	D	1581	NAP	O4D-C1D	3.49	1.45	1.41
2	L	1581	NAP	C3N-C7N	3.51	1.56	1.50
2	N	1581	NAP	C6N-N1N	3.55	1.45	1.35
2	K	1581	NAP	C3N-C7N	3.55	1.56	1.50
2	E	1581	NAP	C3N-C7N	3.55	1.56	1.50
2	F	1581	NAP	C6N-N1N	3.56	1.45	1.35
2	I	1581	NAP	C3N-C7N	3.59	1.56	1.50
2	I	1581	NAP	O4D-C1D	3.61	1.45	1.41
2	C	1581	NAP	C3N-C7N	3.64	1.56	1.50
2	N	1581	NAP	O4D-C1D	3.65	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1581	NAP	O4B-C1B	3.66	1.45	1.41
2	N	1581	NAP	C2A-N3A	3.75	1.38	1.32
2	K	1581	NAP	O4D-C1D	3.76	1.46	1.41
2	I	1581	NAP	O4B-C1B	3.78	1.46	1.41
2	I	1581	NAP	C6N-N1N	3.86	1.45	1.35
2	B	1581	NAP	O4B-C1B	3.92	1.46	1.41
2	G	1581	NAP	O4B-C1B	3.96	1.46	1.41
2	M	1581	NAP	O4B-C1B	4.05	1.46	1.41
2	A	1581	NAP	O4D-C1D	4.05	1.46	1.41
2	C	1581	NAP	O4D-C1D	4.09	1.46	1.41
2	N	1581	NAP	O4B-C1B	4.10	1.46	1.41
2	C	1581	NAP	O4B-C1B	4.15	1.46	1.41
2	H	1581	NAP	O4B-C1B	4.17	1.46	1.41
2	E	1581	NAP	O4D-C1D	4.20	1.46	1.41
2	G	1581	NAP	O4D-C1D	4.24	1.46	1.41
2	D	1581	NAP	O4B-C1B	4.25	1.46	1.41
2	J	1581	NAP	O4D-C1D	4.43	1.46	1.41
2	H	1581	NAP	O4D-C1D	4.74	1.47	1.41
2	O	1581	NAP	O4D-C1D	4.89	1.47	1.41
2	L	1581	NAP	O4B-C1B	4.95	1.47	1.41
2	A	1581	NAP	O4B-C1B	4.95	1.47	1.41
2	K	1581	NAP	O4B-C1B	5.21	1.47	1.41

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1581	NAP	N3A-C2A-N1A	-11.45	120.13	128.89
2	J	1581	NAP	N3A-C2A-N1A	-11.11	120.39	128.89
2	G	1581	NAP	N3A-C2A-N1A	-11.06	120.43	128.89
2	L	1581	NAP	N3A-C2A-N1A	-11.00	120.47	128.89
2	H	1581	NAP	N3A-C2A-N1A	-10.96	120.50	128.89
2	O	1581	NAP	N3A-C2A-N1A	-10.90	120.55	128.89
2	A	1581	NAP	N3A-C2A-N1A	-10.87	120.57	128.89
2	E	1581	NAP	N3A-C2A-N1A	-10.85	120.59	128.89
2	F	1581	NAP	N3A-C2A-N1A	-10.84	120.59	128.89
2	K	1581	NAP	N3A-C2A-N1A	-10.78	120.64	128.89
2	I	1581	NAP	N3A-C2A-N1A	-10.75	120.66	128.89
2	P	1581	NAP	N3A-C2A-N1A	-10.74	120.67	128.89
2	N	1581	NAP	N3A-C2A-N1A	-10.71	120.69	128.89
2	M	1581	NAP	N3A-C2A-N1A	-10.52	120.84	128.89
2	B	1581	NAP	N3A-C2A-N1A	-10.47	120.88	128.89
2	C	1581	NAP	N3A-C2A-N1A	-10.43	120.91	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1581	NAP	C4B-O4B-C1B	-3.79	105.55	109.72
2	I	1581	NAP	C4B-O4B-C1B	-3.78	105.56	109.72
2	J	1581	NAP	C4B-O4B-C1B	-3.72	105.63	109.72
2	L	1581	NAP	C4B-O4B-C1B	-3.68	105.68	109.72
2	K	1581	NAP	C4B-O4B-C1B	-3.67	105.69	109.72
2	C	1581	NAP	C4B-O4B-C1B	-3.66	105.69	109.72
2	O	1581	NAP	C4B-O4B-C1B	-3.49	105.89	109.72
2	B	1581	NAP	C4B-O4B-C1B	-3.43	105.95	109.72
2	D	1581	NAP	C4B-O4B-C1B	-3.34	106.05	109.72
2	P	1581	NAP	C4B-O4B-C1B	-3.28	106.12	109.72
2	G	1581	NAP	C4B-O4B-C1B	-3.23	106.17	109.72
2	F	1581	NAP	C4B-O4B-C1B	-3.04	106.38	109.72
2	A	1581	NAP	C4B-O4B-C1B	-3.03	106.39	109.72
2	M	1581	NAP	C4B-O4B-C1B	-3.02	106.40	109.72
2	O	1581	NAP	C4D-O4D-C1D	-3.01	106.41	109.72
2	E	1581	NAP	C4B-O4B-C1B	-2.99	106.43	109.72
2	H	1581	NAP	C4D-O4D-C1D	-2.96	106.47	109.72
2	I	1581	NAP	C4D-O4D-C1D	-2.70	106.75	109.72
2	F	1581	NAP	C4D-O4D-C1D	-2.59	106.87	109.72
2	C	1581	NAP	C3N-C7N-N7N	-2.43	115.16	117.82
2	N	1581	NAP	C4D-O4D-C1D	-2.41	107.07	109.72
2	E	1581	NAP	C3N-C7N-N7N	-2.37	115.22	117.82
2	J	1581	NAP	C4D-O4D-C1D	-2.37	107.11	109.72
2	K	1581	NAP	C3N-C7N-N7N	-2.34	115.26	117.82
2	P	1581	NAP	C3N-C7N-N7N	-2.33	115.27	117.82
2	H	1581	NAP	C4B-O4B-C1B	-2.33	107.16	109.72
2	J	1581	NAP	C1B-N9A-C4A	-2.33	123.43	126.94
2	B	1581	NAP	C4D-O4D-C1D	-2.28	107.21	109.72
2	H	1581	NAP	C3N-C7N-N7N	-2.25	115.35	117.82
2	D	1581	NAP	C4D-O4D-C1D	-2.23	107.27	109.72
2	M	1581	NAP	C3N-C7N-N7N	-2.20	115.40	117.82
2	D	1581	NAP	C1B-N9A-C4A	-2.17	123.67	126.94
2	F	1581	NAP	C3N-C7N-N7N	-2.16	115.45	117.82
2	G	1581	NAP	C3N-C7N-N7N	-2.16	115.45	117.82
2	J	1581	NAP	C3N-C7N-N7N	-2.12	115.50	117.82
2	M	1581	NAP	C4D-O4D-C1D	-2.11	107.40	109.72
2	N	1581	NAP	C3N-C7N-N7N	-2.10	115.52	117.82
2	B	1581	NAP	C3N-C7N-N7N	-2.10	115.52	117.82
2	I	1581	NAP	C1B-N9A-C4A	-2.09	123.79	126.94
2	K	1581	NAP	C4D-O4D-C1D	-2.07	107.45	109.72
2	P	1581	NAP	C4D-O4D-C1D	-2.05	107.46	109.72
2	L	1581	NAP	C3N-C7N-N7N	-2.00	115.62	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1581	NAP	O4B-C1B-N9A	2.16	112.62	108.10
2	O	1581	NAP	O4B-C1B-N9A	2.20	112.71	108.10
2	B	1581	NAP	O4B-C1B-N9A	2.35	113.02	108.10
2	N	1581	NAP	O4B-C1B-N9A	2.43	113.18	108.10
2	I	1581	NAP	O4B-C1B-N9A	2.53	113.39	108.10
2	F	1581	NAP	O4B-C1B-N9A	2.54	113.41	108.10
2	C	1581	NAP	O4D-C1D-N1N	2.77	111.17	108.13
2	P	1581	NAP	O4D-C1D-N1N	3.32	111.78	108.13
2	M	1581	NAP	O4D-C1D-N1N	3.39	111.86	108.13
2	B	1581	NAP	O4D-C1D-N1N	3.50	111.98	108.13
2	N	1581	NAP	O4D-C1D-N1N	3.58	112.07	108.13
2	J	1581	NAP	O4D-C1D-N1N	3.64	112.12	108.13
2	L	1581	NAP	O4D-C1D-N1N	3.64	112.13	108.13
2	K	1581	NAP	O4D-C1D-N1N	3.67	112.16	108.13
2	E	1581	NAP	O4D-C1D-N1N	3.68	112.18	108.13
2	F	1581	NAP	O4D-C1D-N1N	3.75	112.26	108.13
2	G	1581	NAP	O4D-C1D-N1N	3.77	112.27	108.13
2	A	1581	NAP	O4D-C1D-N1N	3.79	112.29	108.13
2	D	1581	NAP	O4D-C1D-N1N	3.89	112.41	108.13
2	I	1581	NAP	O4D-C1D-N1N	3.91	112.43	108.13
2	O	1581	NAP	O4D-C1D-N1N	4.19	112.73	108.13
2	H	1581	NAP	O4D-C1D-N1N	4.30	112.86	108.13
2	H	1581	NAP	C4A-C5A-N7A	4.41	113.53	109.48
2	B	1581	NAP	C4A-C5A-N7A	4.41	113.54	109.48
2	M	1581	NAP	C4A-C5A-N7A	4.42	113.54	109.48
2	C	1581	NAP	C4A-C5A-N7A	4.42	113.54	109.48
2	L	1581	NAP	C4A-C5A-N7A	4.46	113.58	109.48
2	N	1581	NAP	C4A-C5A-N7A	4.49	113.61	109.48
2	F	1581	NAP	C4A-C5A-N7A	4.49	113.61	109.48
2	P	1581	NAP	C4A-C5A-N7A	4.50	113.62	109.48
2	J	1581	NAP	C4A-C5A-N7A	4.53	113.64	109.48
2	I	1581	NAP	C4A-C5A-N7A	4.53	113.64	109.48
2	K	1581	NAP	C4A-C5A-N7A	4.63	113.73	109.48
2	D	1581	NAP	C4A-C5A-N7A	4.65	113.76	109.48
2	G	1581	NAP	C4A-C5A-N7A	4.66	113.76	109.48
2	E	1581	NAP	C4A-C5A-N7A	4.66	113.77	109.48
2	O	1581	NAP	C4A-C5A-N7A	4.74	113.84	109.48
2	A	1581	NAP	C4A-C5A-N7A	4.79	113.88	109.48
2	O	1581	NAP	P2B-O2B-C2B	5.14	133.89	121.56
2	D	1581	NAP	P2B-O2B-C2B	5.23	134.10	121.56
2	B	1581	NAP	P2B-O2B-C2B	5.28	134.23	121.56
2	F	1581	NAP	P2B-O2B-C2B	5.29	134.25	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1581	NAP	P2B-O2B-C2B	5.30	134.27	121.56
2	G	1581	NAP	P2B-O2B-C2B	5.35	134.40	121.56
2	M	1581	NAP	P2B-O2B-C2B	5.42	134.56	121.56
2	I	1581	NAP	P2B-O2B-C2B	5.51	134.77	121.56
2	L	1581	NAP	P2B-O2B-C2B	5.61	135.02	121.56
2	P	1581	NAP	P2B-O2B-C2B	5.66	135.15	121.56
2	C	1581	NAP	P2B-O2B-C2B	5.69	135.20	121.56
2	K	1581	NAP	P2B-O2B-C2B	5.70	135.22	121.56
2	H	1581	NAP	P2B-O2B-C2B	5.76	135.37	121.56
2	A	1581	NAP	P2B-O2B-C2B	5.78	135.43	121.56
2	N	1581	NAP	P2B-O2B-C2B	5.80	135.47	121.56
2	E	1581	NAP	P2B-O2B-C2B	5.84	135.58	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1581	NAP	4	0
3	A	1583	OXL	1	0
2	B	1581	NAP	4	0
3	B	1582	OXL	1	0
2	C	1581	NAP	2	0
3	C	1582	OXL	3	0
2	D	1581	NAP	2	0
3	D	1582	OXL	2	0
2	E	1581	NAP	3	0
3	E	1582	OXL	1	0
2	F	1581	NAP	2	0
3	F	1582	OXL	1	0
2	G	1581	NAP	3	0
3	G	1582	OXL	1	0
2	H	1581	NAP	3	0
3	H	1582	OXL	1	0
2	I	1581	NAP	3	0
2	J	1581	NAP	4	0
3	J	1582	OXL	1	0
2	K	1581	NAP	5	0
3	K	1582	OXL	1	0
2	L	1581	NAP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1582	OXL	1	0
2	M	1581	NAP	3	0
2	N	1581	NAP	3	0
3	N	1582	OXL	1	0
2	O	1581	NAP	2	0
2	P	1581	NAP	1	0
3	P	1582	OXL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.