



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 PM GMT

PDB ID : 3WST  
Title : Crystal structure of C.elegans PRMT7 in complex with SAH(P31)  
Authors : Hasegawa, M.; Toma-fukai, S.; Shimizu, T.  
Deposited on : 2014-03-21  
Resolution : 2.39 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

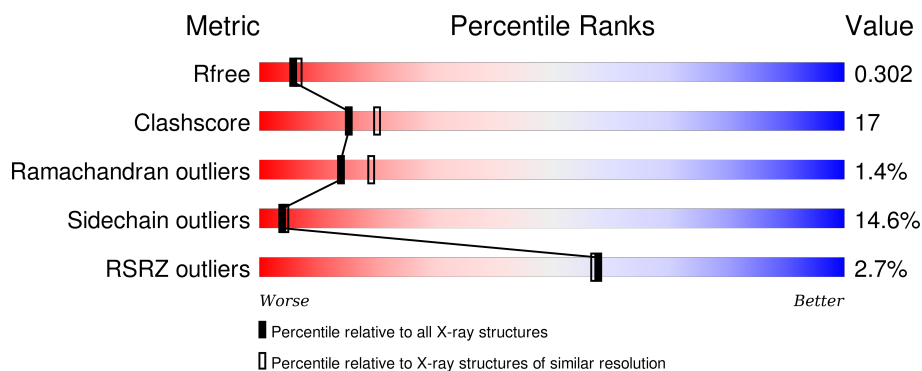
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	655	 69% 23% 6% •
1	B	655	 61% 29% 8% •
1	C	655	 63% 30% • •
1	D	655	 69% 24% • •
1	E	655	 62% 27% 7% •

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Mol	Chain	Length	Quality of chain
1	F	655	
1	G	655	
1	H	655	
1	I	655	
1	J	655	
1	K	655	
1	L	655	
1	M	655	
1	N	655	
1	O	655	
1	P	655	
1	Q	655	
1	R	655	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	D	637	Total	C	N	O	S	0	0	0
			5078	3231	852	968	27			
1	B	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	C	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	F	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	E	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	G	636	Total	C	N	O	S	0	0	0
			5070	3227	850	966	27			
1	H	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	I	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			
1	M	633	Total	C	N	O	S	0	0	0
			5049	3216	844	962	27			
1	N	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	O	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	P	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	Q	632	Total	C	N	O	S	0	0	0
			5039	3209	845	958	27			
1	R	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	J	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	L	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
A	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
A	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
A	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
A	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
D	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
D	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
D	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
D	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
D	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
B	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
B	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
B	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
B	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
B	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
C	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
C	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
C	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
C	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
C	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
F	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
F	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
F	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
F	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
E	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
E	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
E	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
E	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
E	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
G	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
G	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
G	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
G	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
G	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
H	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
H	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
H	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
H	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
H	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
I	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
I	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
I	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
I	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
I	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
M	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
M	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
M	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
M	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
M	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
M	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
M	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
N	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
N	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
N	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
N	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
N	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
O	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
O	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
O	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
O	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
O	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
P	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
P	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
P	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
P	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
P	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
Q	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
Q	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
Q	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
Q	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
Q	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
R	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
R	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
R	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
R	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
R	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
R	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42

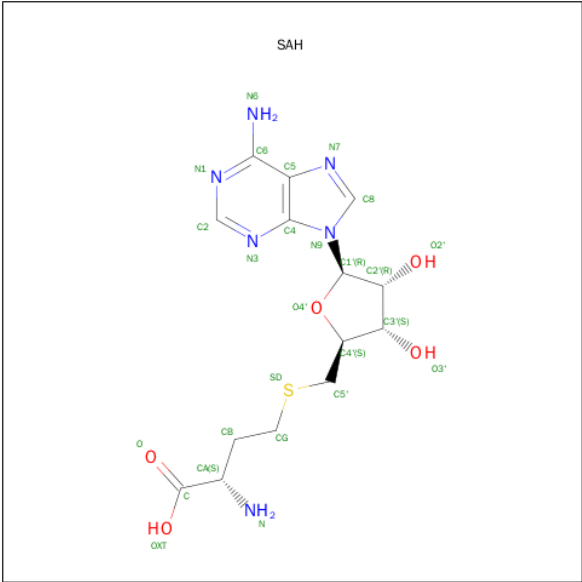
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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
R	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
J	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
J	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
J	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
J	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
J	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
K	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
K	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
K	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
K	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
K	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
L	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
L	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
L	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
L	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
L	0	PRO	-	EXPRESSION TAG	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).





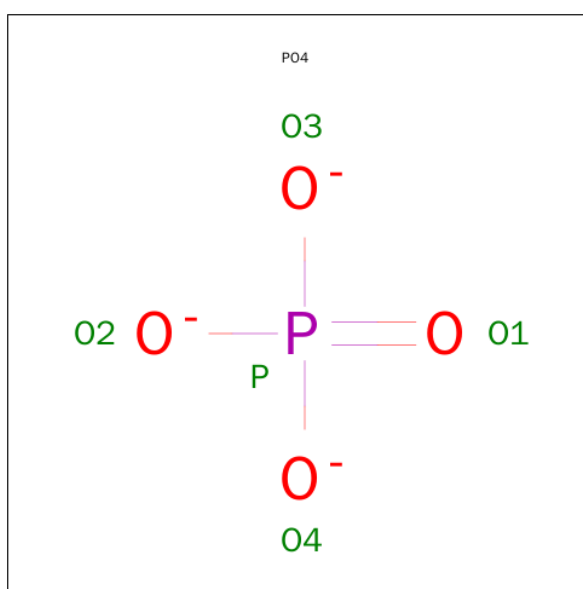
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	N	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	O	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	P	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	Q	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	D	93	Total	O	0	0
			93	93		
4	B	26	Total	O	0	0
			26	26		
4	C	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		
4	E	41	Total	O	0	0
			41	41		
4	G	19	Total	O	0	0
			19	19		
4	H	59	Total	O	0	0
			59	59		

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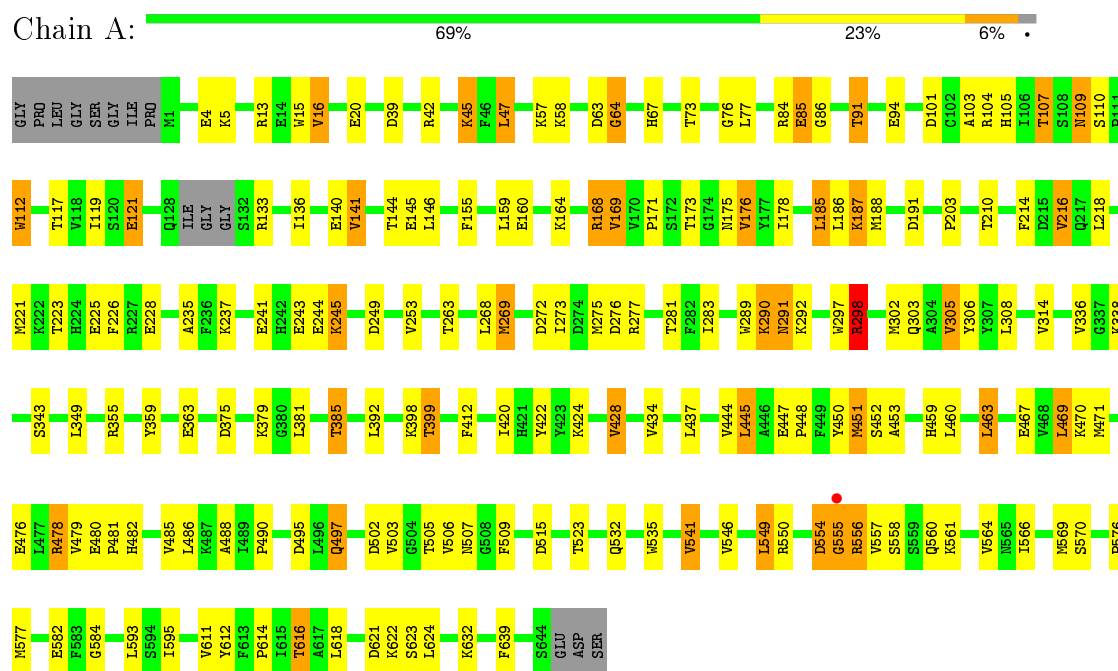
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	21	Total 21	O 21	0	0
4	M	2	Total 2	O 2	0	0
4	P	10	Total 10	O 10	0	0
4	Q	2	Total 2	O 2	0	0
4	R	2	Total 2	O 2	0	0
4	J	12	Total 12	O 12	0	0
4	K	6	Total 6	O 6	0	0
4	L	85	Total 85	O 85	0	0

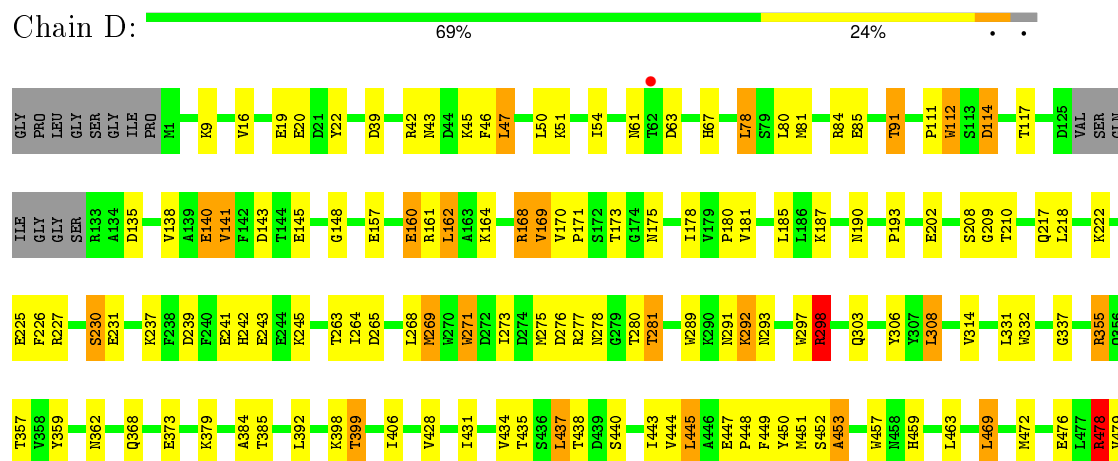
### 3 Residue-property plots

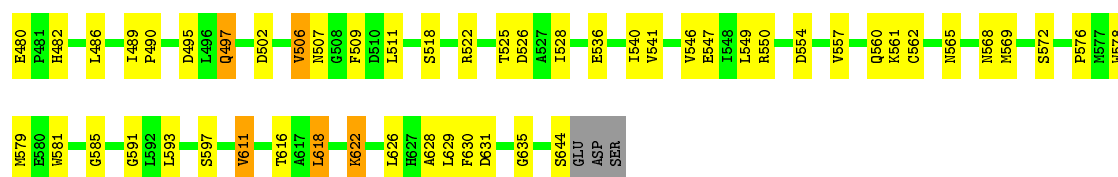
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Protein arginine N-methyltransferase 7

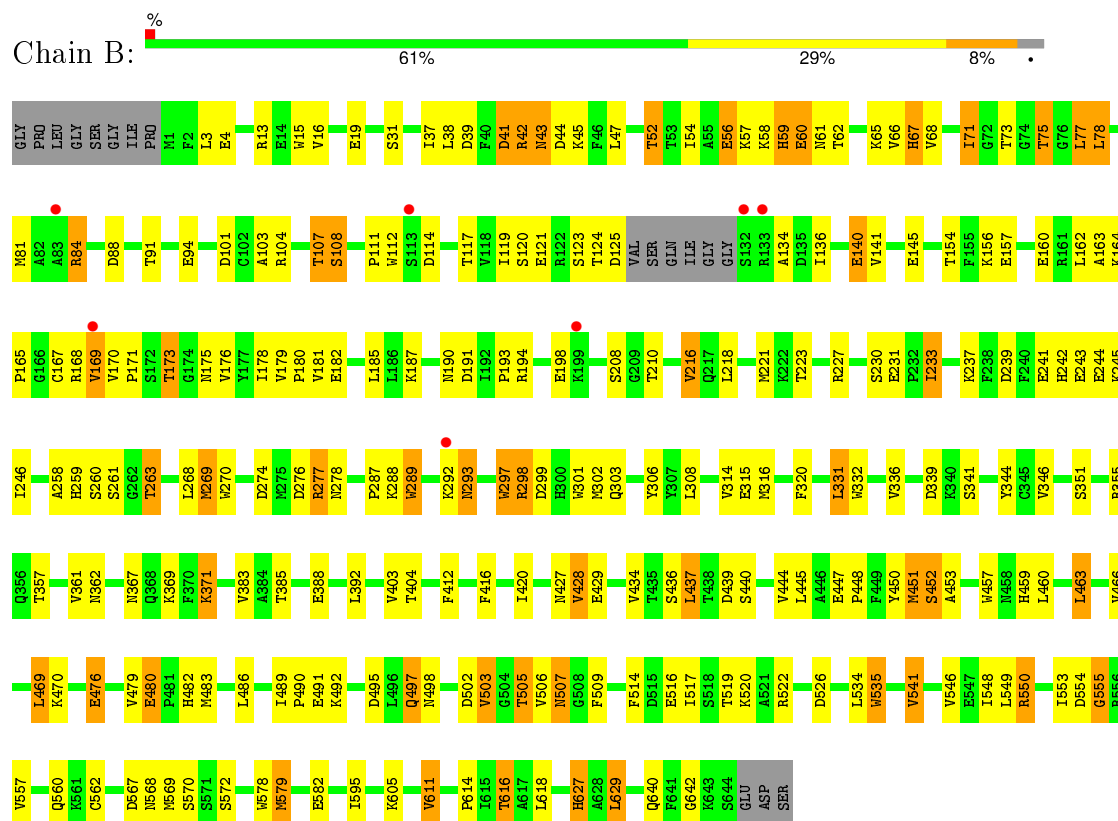


#### • Molecule 1: Protein arginine N-methyltransferase 7

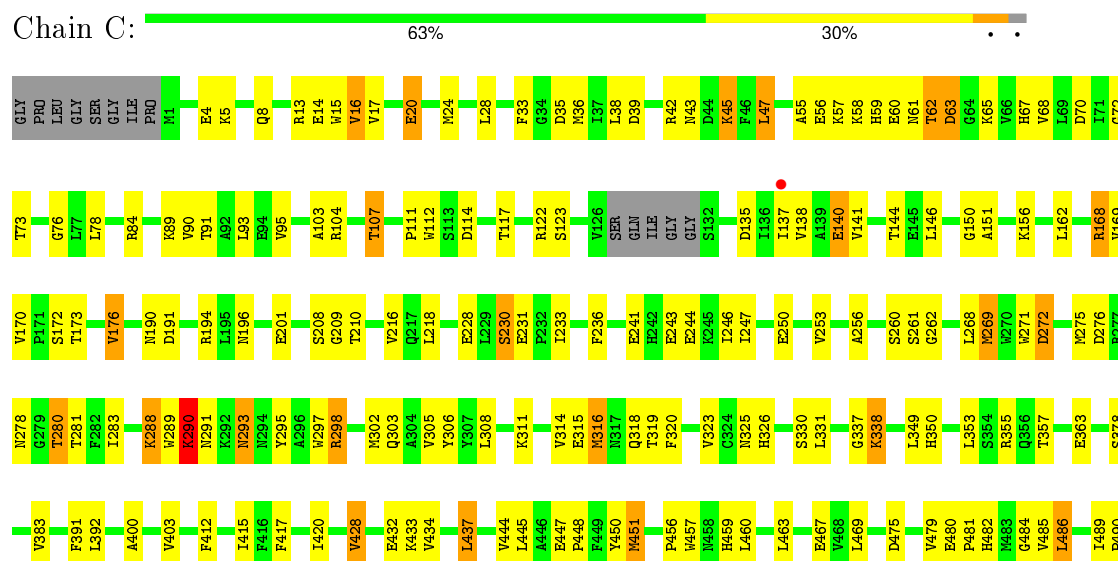


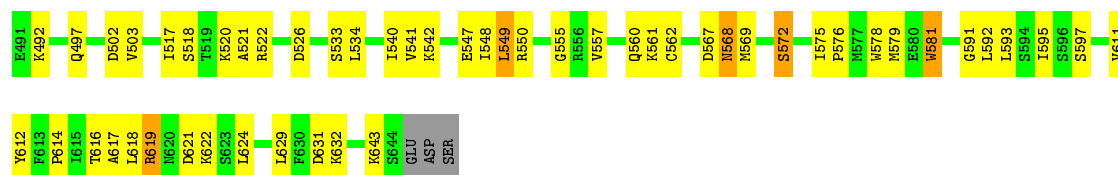


• Molecule 1: Protein arginine N-methyltransferase 7

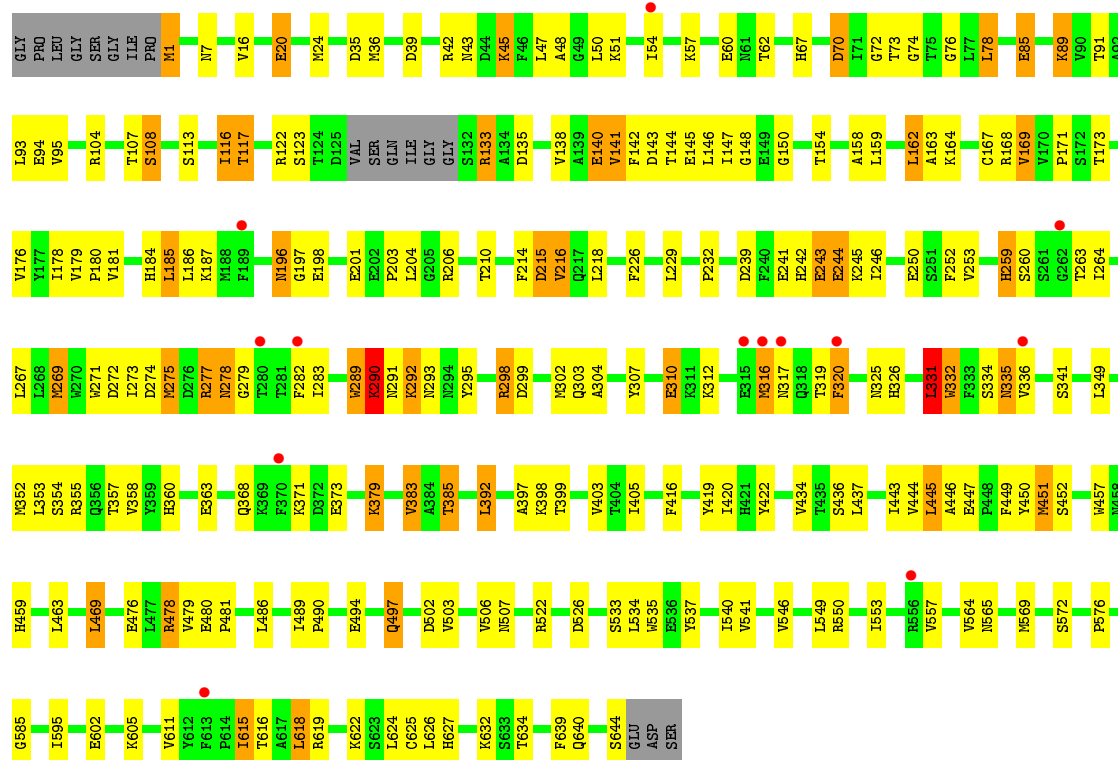


• Molecule 1: Protein arginine N-methyltransferase 7

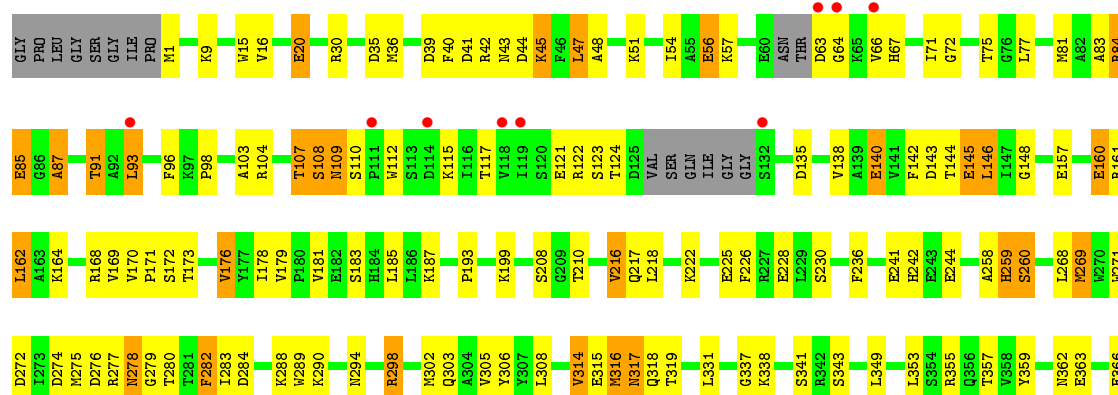


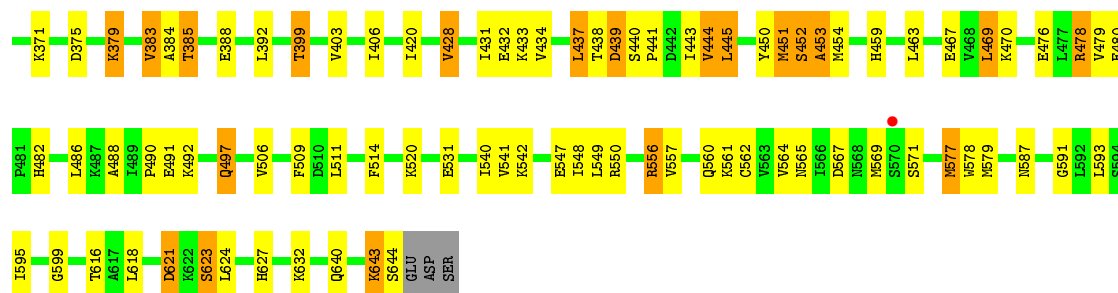


• Molecule 1: Protein arginine N-methyltransferase 7

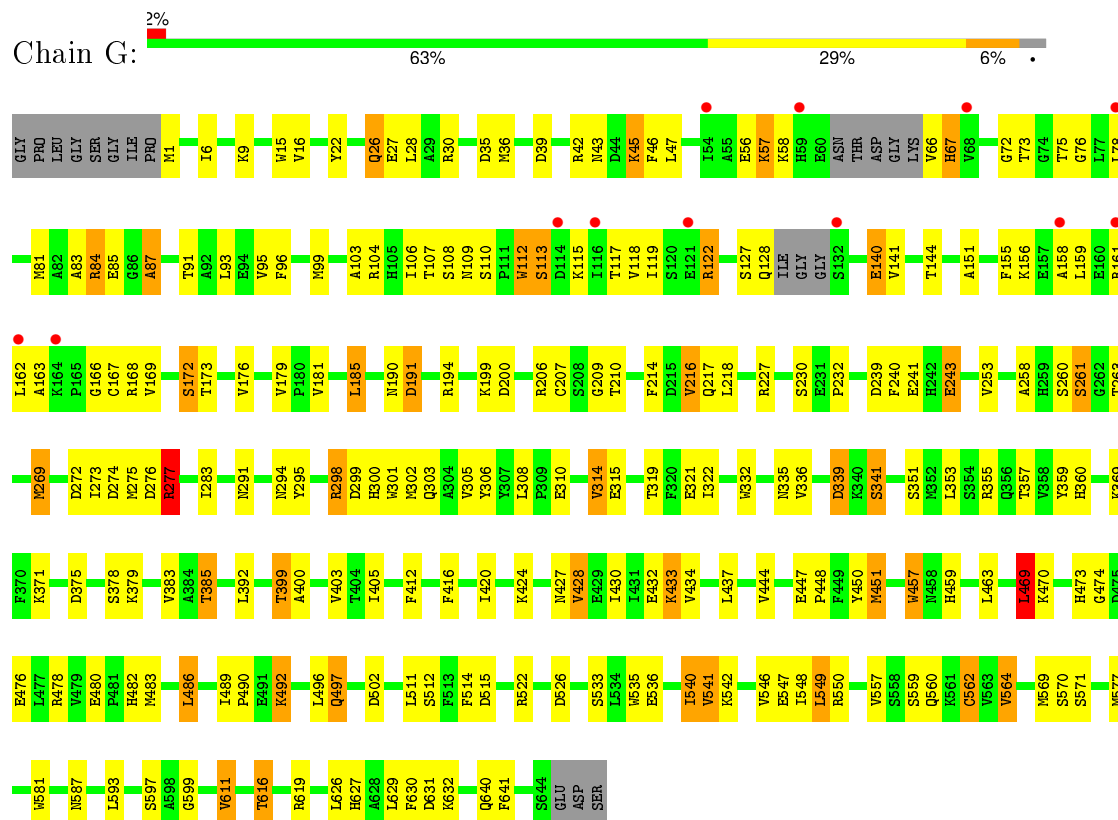


• Molecule 1: Protein arginine N-methyltransferase 7

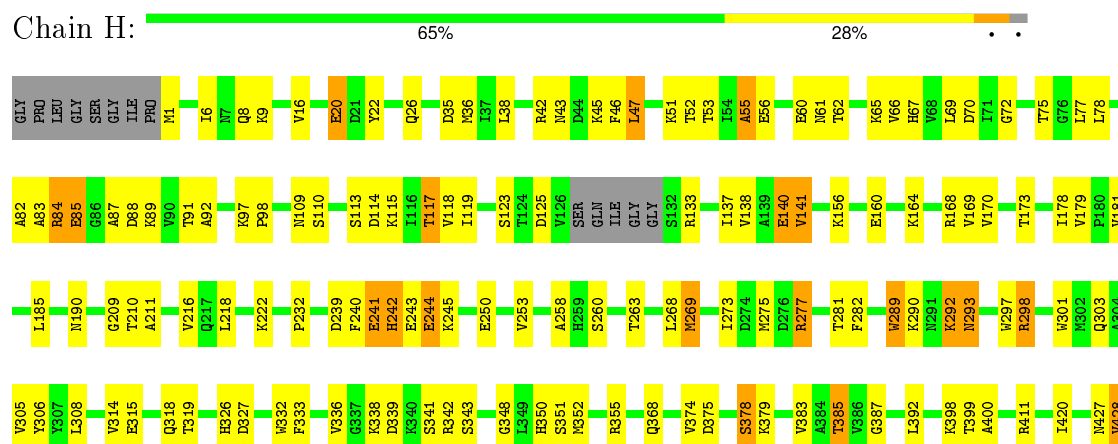




• Molecule 1: Protein arginine N-methyltransferase 7



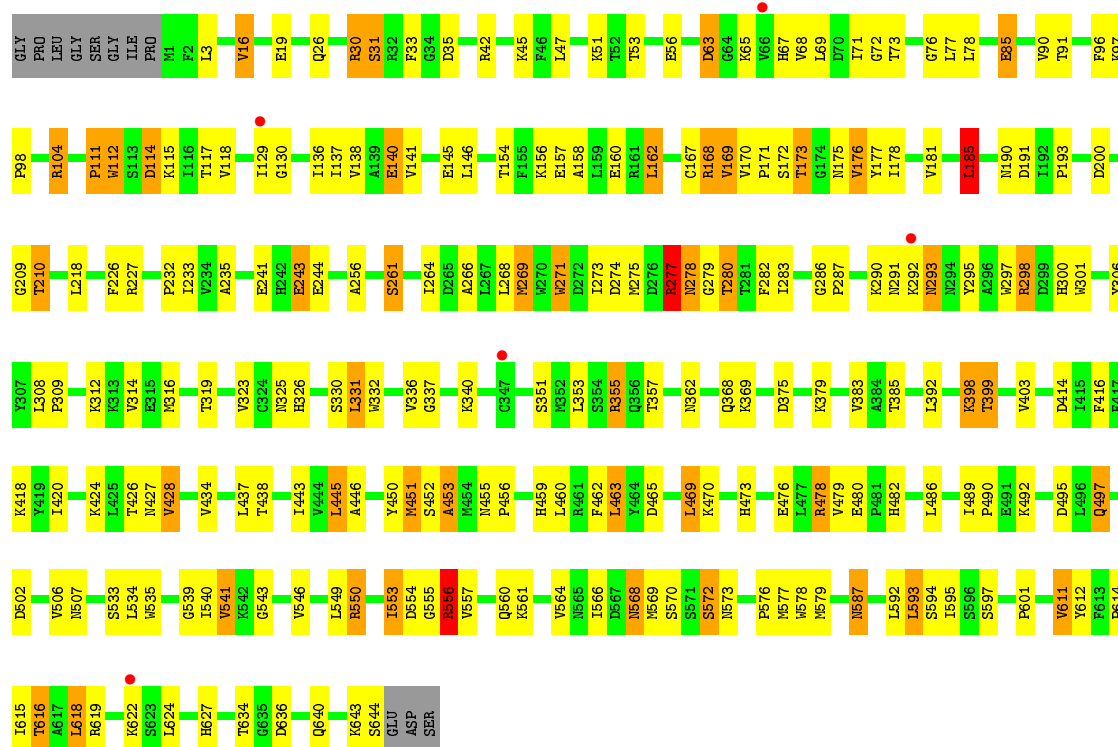
• Molecule 1: Protein arginine N-methyltransferase 7



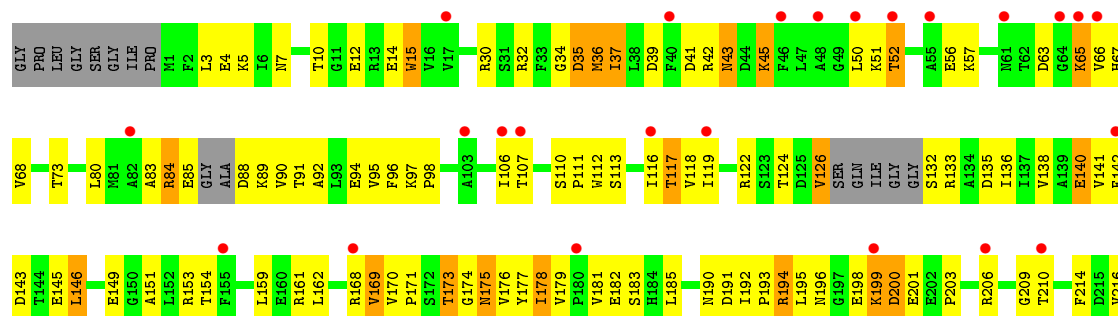


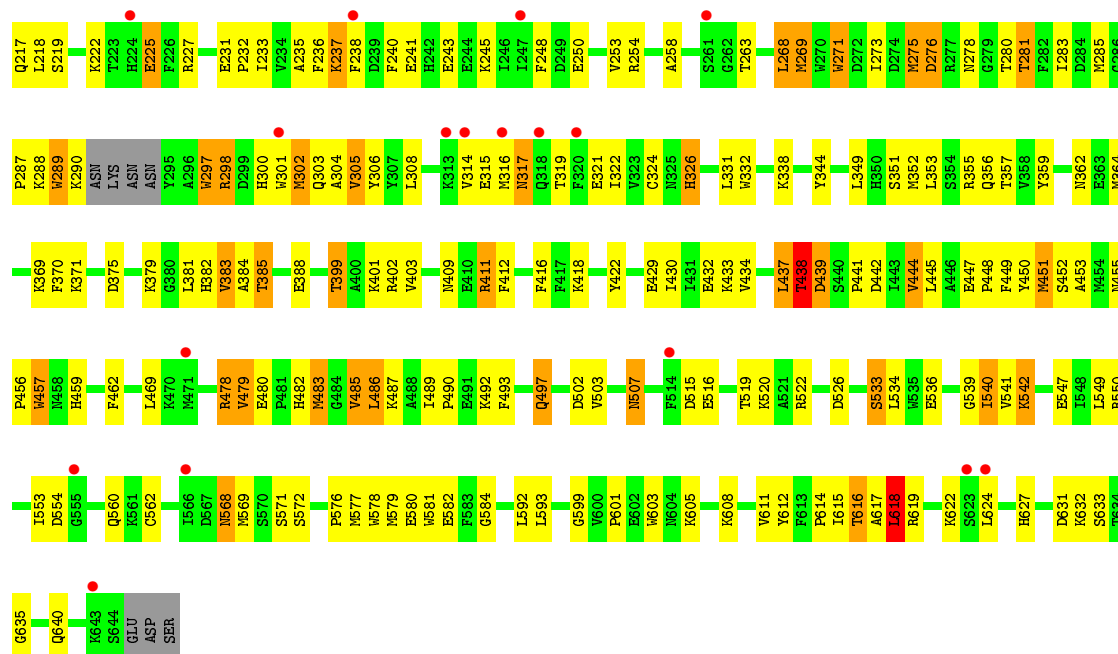


• Molecule 1: Protein arginine N-methyltransferase 7

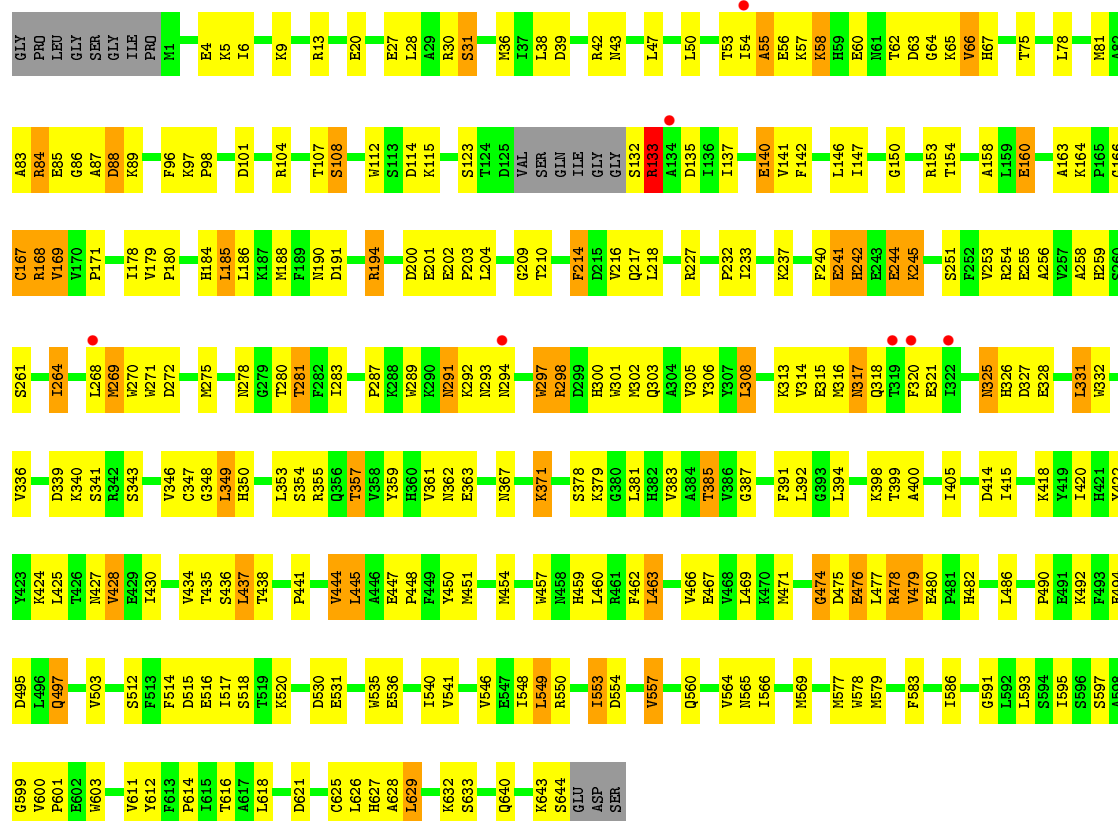


• Molecule 1: Protein arginine N-methyltransferase 7

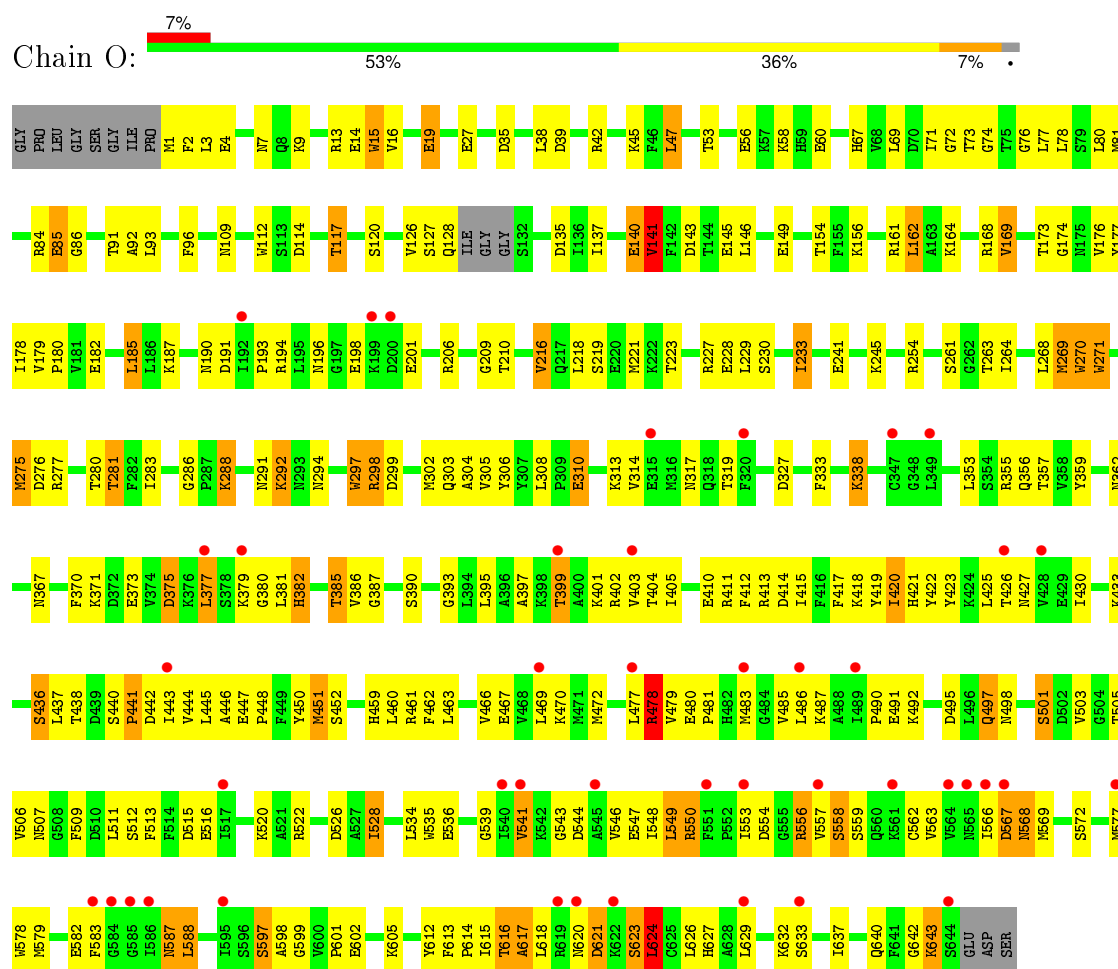


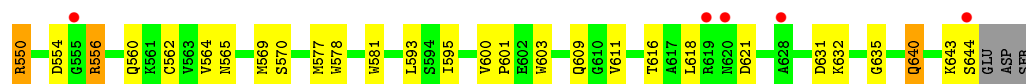


• Molecule 1: Protein arginine N-methyltransferase 7

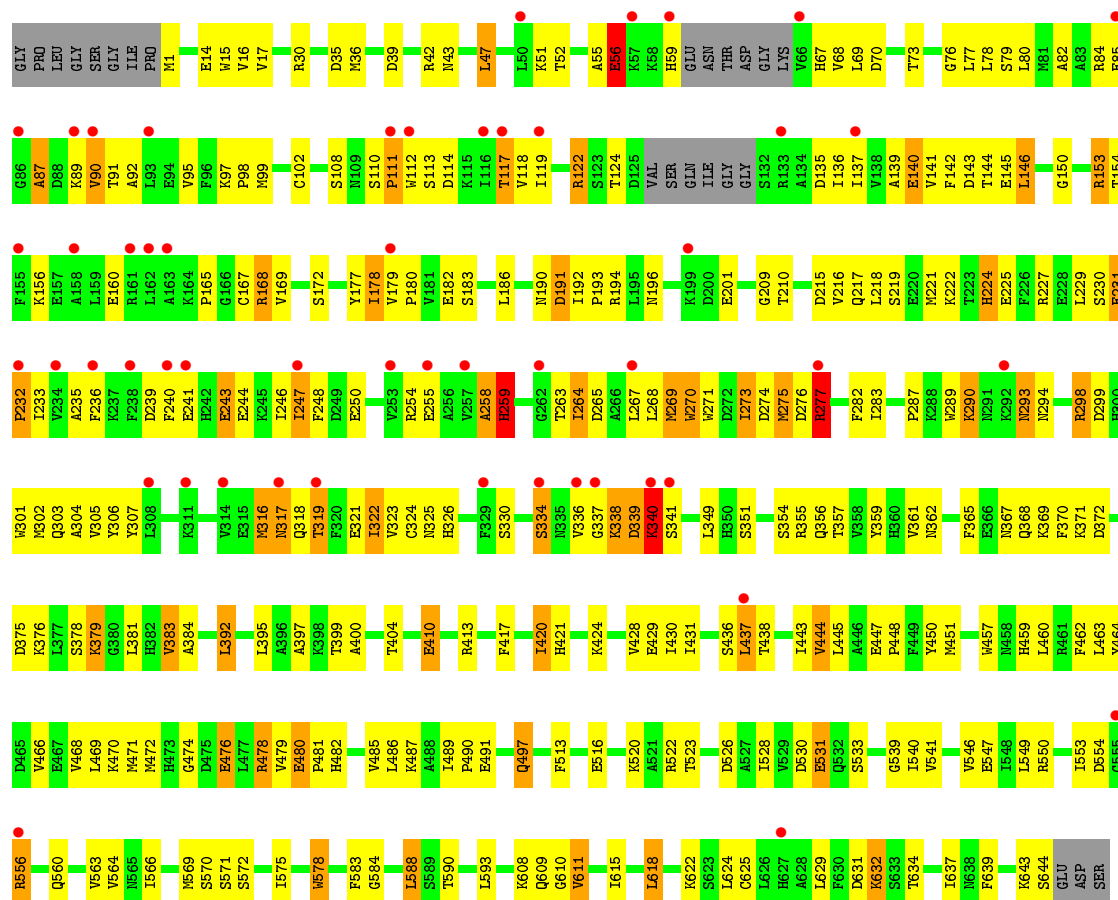


• Molecule 1: Protein arginine N-methyltransferase 7

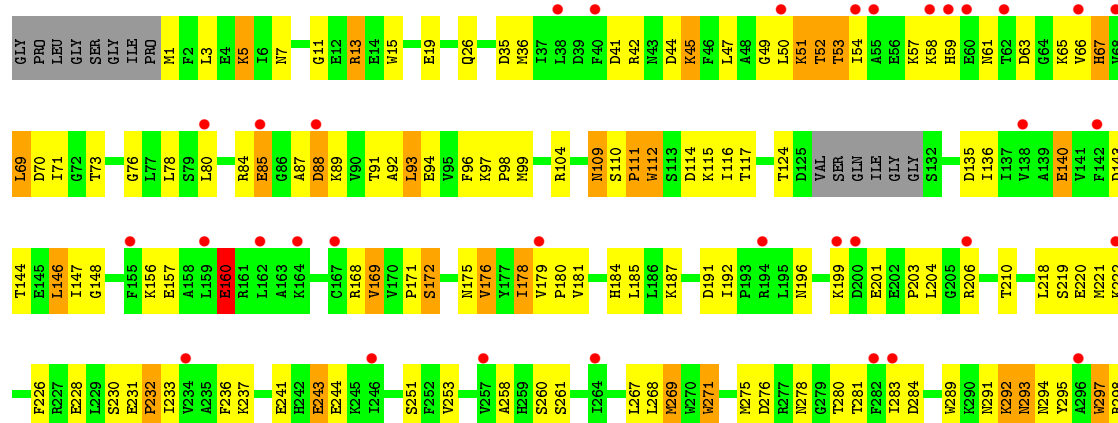


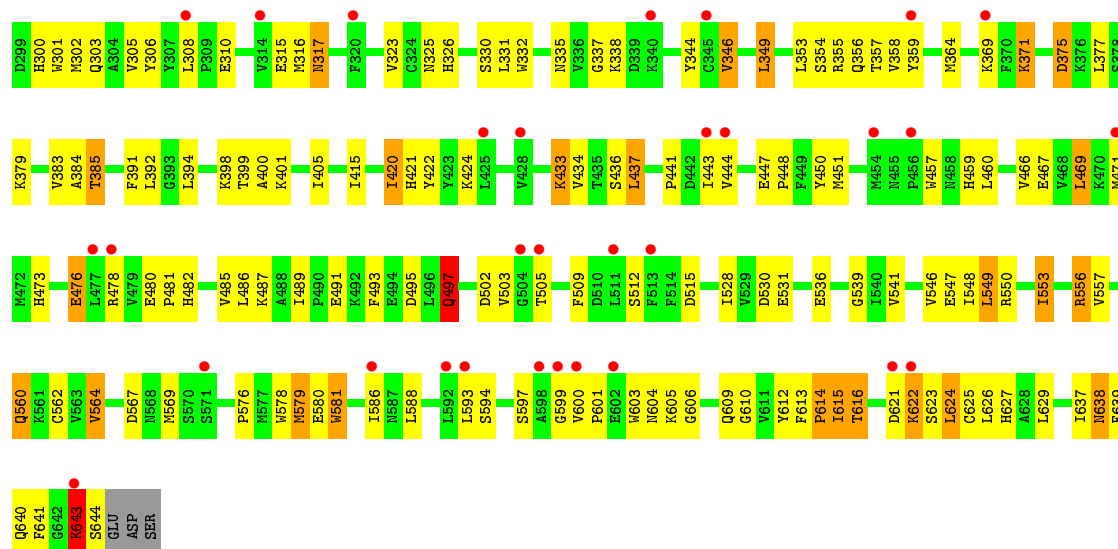


• Molecule 1: Protein arginine N-methyltransferase 7

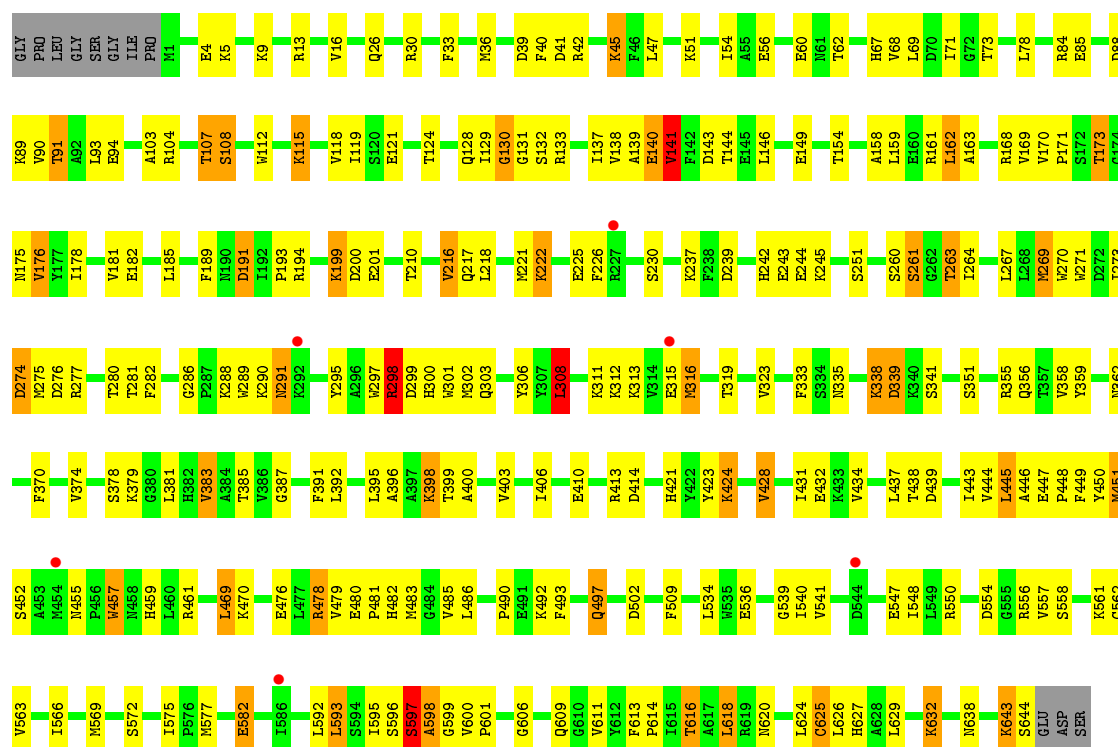


• Molecule 1: Protein arginine N-methyltransferase 7



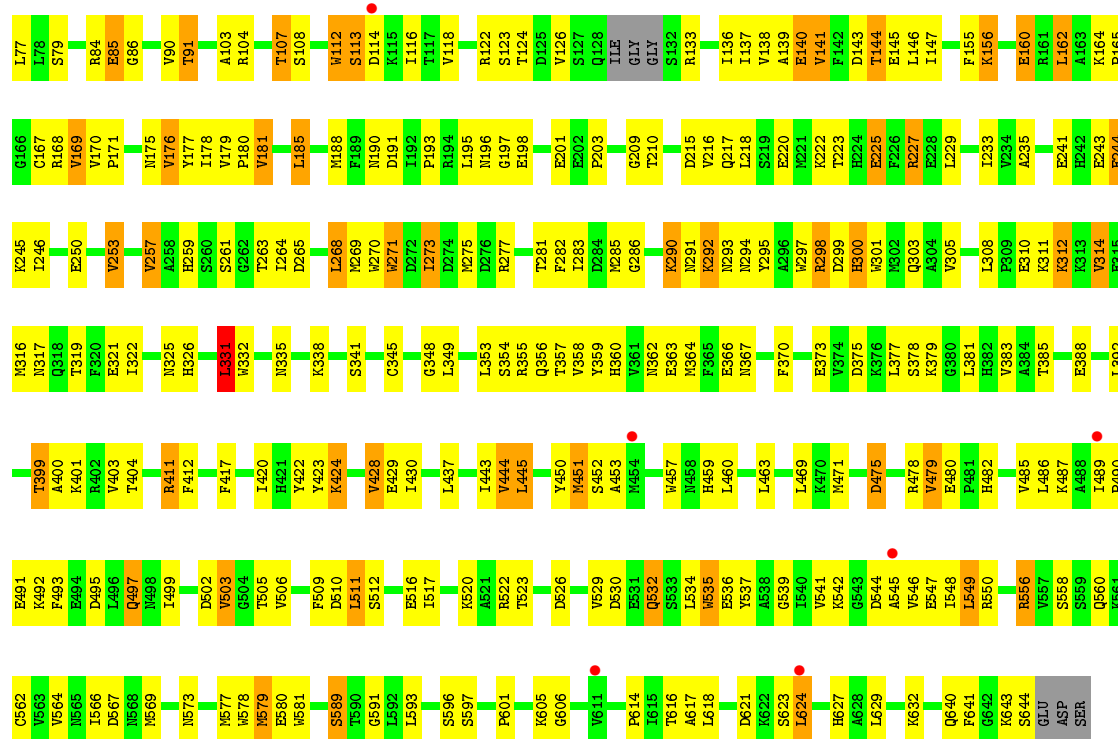


• Molecule 1: Protein arginine N-methyltransferase 7



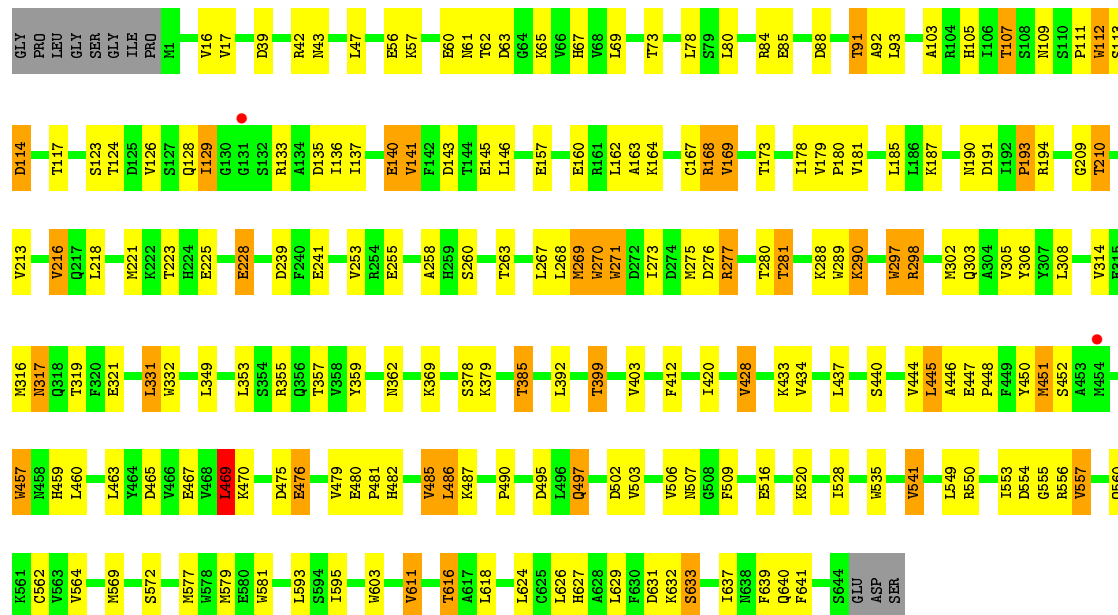
• Molecule 1: Protein arginine N-methyltransferase 7





### • Molecule 1: Protein arginine N-methyltransferase 7

Chain L: 68% 25% 6% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 2.39 47.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.41-2.39) 98.9 (47.41-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.234 , 0.303 0.233 , 0.302	Depositor DCC
$R_{free}$ test set	29764 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 15.4	EDS
Estimated twinning fraction	0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 593388 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	92645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SAH

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	0.85	4/5217 (0.1%)	0.95	5/7044 (0.1%)
1	B	0.79	7/5195 (0.1%)	0.88	0/7014
1	C	0.77	2/5202 (0.0%)	0.88	3/7024 (0.0%)
1	D	0.81	6/5189 (0.1%)	0.96	8/7006 (0.1%)
1	E	0.79	2/5179 (0.0%)	0.94	3/6990 (0.0%)
1	F	0.73	4/5195 (0.1%)	0.88	7/7014 (0.1%)
1	G	0.77	6/5180 (0.1%)	0.90	5/6993 (0.1%)
1	H	0.81	5/5202 (0.1%)	0.92	3/7024 (0.0%)
1	I	0.76	4/5234 (0.1%)	0.86	3/7068 (0.0%)
1	J	0.74	2/5234 (0.0%)	0.88	6/7068 (0.1%)
1	K	0.73	4/5217 (0.1%)	0.85	5/7044 (0.1%)
1	L	0.86	9/5234 (0.2%)	0.99	8/7068 (0.1%)
1	M	0.70	7/5158 (0.1%)	0.81	3/6962 (0.0%)
1	N	0.70	4/5195 (0.1%)	0.84	4/7014 (0.1%)
1	O	0.66	5/5217 (0.1%)	0.78	3/7044 (0.0%)
1	P	0.74	7/5179 (0.1%)	0.85	4/6990 (0.1%)
1	Q	0.68	5/5149 (0.1%)	0.81	1/6951 (0.0%)
1	R	0.65	8/5195 (0.2%)	0.77	0/7014
All	All	0.76	91/93571 (0.1%)	0.88	71/126332 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	H	0	1
1	J	0	2
All	All	0	6



All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	332	TRP	CD2-CE2	7.16	1.50	1.41
1	M	271	TRP	CD2-CE2	6.90	1.49	1.41
1	L	297	TRP	CD2-CE2	6.63	1.49	1.41
1	D	332	TRP	CD2-CE2	6.55	1.49	1.41
1	A	289	TRP	CD2-CE2	6.37	1.49	1.41
1	H	332	TRP	CD2-CE2	6.34	1.49	1.41
1	P	578	TRP	CD2-CE2	6.32	1.49	1.41
1	G	535	TRP	CD2-CE2	6.27	1.48	1.41
1	A	535	TRP	CD2-CE2	6.25	1.48	1.41
1	O	271	TRP	CD2-CE2	6.18	1.48	1.41
1	D	581	TRP	CD2-CE2	6.16	1.48	1.41
1	M	581	TRP	CD2-CE2	6.15	1.48	1.41
1	G	581	TRP	CD2-CE2	6.11	1.48	1.41
1	B	578	TRP	CD2-CE2	6.10	1.48	1.41
1	G	457	TRP	CD2-CE2	6.09	1.48	1.41
1	B	270	TRP	CD2-CE2	6.08	1.48	1.41
1	H	457	TRP	CD2-CE2	6.04	1.48	1.41
1	E	289	TRP	CD2-CE2	6.04	1.48	1.41
1	F	457	TRP	CD2-CE2	6.00	1.48	1.41
1	L	535	TRP	CD2-CE2	5.99	1.48	1.41
1	J	457	TRP	CD2-CE2	5.97	1.48	1.41
1	R	603	TRP	CD2-CE2	5.94	1.48	1.41
1	G	332	TRP	CD2-CE2	5.93	1.48	1.41
1	K	332	TRP	CD2-CE2	5.92	1.48	1.41
1	K	457	TRP	CD2-CE2	5.83	1.48	1.41
1	P	535	TRP	CD2-CE2	5.79	1.48	1.41
1	Q	578	TRP	CD2-CE2	5.79	1.48	1.41
1	B	289	TRP	CD2-CE2	5.79	1.48	1.41
1	B	332	TRP	CD2-CE2	5.78	1.48	1.41
1	D	289	TRP	CD2-CE2	5.76	1.48	1.41
1	P	457	TRP	CD2-CE2	5.74	1.48	1.41
1	N	270	TRP	CD2-CE2	5.73	1.48	1.41
1	N	603	TRP	CD2-CE2	5.68	1.48	1.41
1	P	603	TRP	CD2-CE2	5.65	1.48	1.41
1	L	112	TRP	CD2-CE2	5.65	1.48	1.41
1	M	457	TRP	CD2-CE2	5.64	1.48	1.41
1	N	457	TRP	CD2-CE2	5.62	1.48	1.41
1	L	289	TRP	CD2-CE2	5.60	1.48	1.41
1	R	581	TRP	CD2-CE2	5.57	1.48	1.41
1	K	581	TRP	CD2-CE2	5.56	1.48	1.41
1	F	332	TRP	CD2-CE2	5.55	1.48	1.41
1	Q	270	TRP	CD2-CE2	5.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	CD2-CE2	5.53	1.48	1.41
1	N	297	TRP	CD2-CE2	5.51	1.48	1.41
1	B	535	TRP	CD2-CE2	5.49	1.48	1.41
1	I	332	TRP	CD2-CE2	5.47	1.48	1.41
1	P	297	TRP	CD2-CE2	5.45	1.47	1.41
1	B	457	TRP	CD2-CE2	5.45	1.47	1.41
1	P	301	TRP	CD2-CE2	5.44	1.47	1.41
1	R	457	TRP	CD2-CE2	5.44	1.47	1.41
1	I	112	TRP	CD2-CE2	5.38	1.47	1.41
1	Q	301	TRP	CD2-CE2	5.38	1.47	1.41
1	M	297	TRP	CD2-CE2	5.36	1.47	1.41
1	H	301	TRP	CD2-CE2	5.34	1.47	1.41
1	R	112	TRP	CD2-CE2	5.34	1.47	1.41
1	L	271	TRP	CD2-CE2	5.34	1.47	1.41
1	G	112	TRP	CD2-CE2	5.33	1.47	1.41
1	M	603	TRP	CD2-CE2	5.33	1.47	1.41
1	H	581	TRP	CD2-CE2	5.32	1.47	1.41
1	G	15	TRP	CD2-CE2	5.31	1.47	1.41
1	P	581	TRP	CD2-CE2	5.31	1.47	1.41
1	A	112	TRP	CD2-CE2	5.30	1.47	1.41
1	Q	15	TRP	CD2-CE2	5.29	1.47	1.41
1	Q	457	TRP	CD2-CE2	5.28	1.47	1.41
1	F	271	TRP	CD2-CE2	5.28	1.47	1.41
1	O	297	TRP	CD2-CE2	5.23	1.47	1.41
1	D	271	TRP	CD2-CE2	5.22	1.47	1.41
1	I	535	TRP	CD2-CE2	5.22	1.47	1.41
1	E	112	TRP	CD2-CE2	5.21	1.47	1.41
1	R	289	TRP	CD2-CE2	5.21	1.47	1.41
1	M	332	TRP	CD2-CE2	5.21	1.47	1.41
1	K	271	TRP	CD2-CE2	5.18	1.47	1.41
1	R	271	TRP	CD2-CE2	5.18	1.47	1.41
1	I	271	TRP	CD2-CE2	5.16	1.47	1.41
1	O	15	TRP	CD2-CE2	5.16	1.47	1.41
1	J	271	TRP	CD2-CE2	5.16	1.47	1.41
1	R	297	TRP	CD2-CE2	5.15	1.47	1.41
1	M	15	TRP	CD2-CE2	5.15	1.47	1.41
1	H	289	TRP	CD2-CE2	5.13	1.47	1.41
1	C	297	TRP	CD2-CE2	5.13	1.47	1.41
1	C	581	TRP	CD2-CE2	5.12	1.47	1.41
1	F	289	TRP	CD2-CE2	5.12	1.47	1.41
1	L	457	TRP	CD2-CE2	5.12	1.47	1.41
1	O	270	TRP	CD2-CE2	5.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	TRP	CD2-CE2	5.09	1.47	1.41
1	L	603	TRP	CD2-CE2	5.07	1.47	1.41
1	O	578	TRP	CD2-CE2	5.05	1.47	1.41
1	L	270	TRP	CD2-CE2	5.05	1.47	1.41
1	B	297	TRP	CD2-CE2	5.04	1.47	1.41
1	D	457	TRP	CD2-CE2	5.03	1.47	1.41
1	R	332	TRP	CD2-CE2	5.03	1.47	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	277	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	F	331	LEU	CA-CB-CG	9.32	136.75	115.30
1	L	611	VAL	CB-CA-C	-8.32	95.60	111.40
1	L	277	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	D	611	VAL	CB-CA-C	-7.93	96.34	111.40
1	K	331	LEU	CA-CB-CG	7.65	132.90	115.30
1	Q	611	VAL	CB-CA-C	-7.34	97.45	111.40
1	J	298	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	E	579	MET	CG-SD-CE	-7.25	88.59	100.20
1	C	437	LEU	CA-CB-CG	7.22	131.91	115.30
1	N	241	GLU	N-CA-C	7.17	130.36	111.00
1	H	611	VAL	CB-CA-C	-6.76	98.55	111.40
1	H	241	GLU	C-N-CA	6.58	138.16	121.70
1	O	624	LEU	CA-CB-CG	6.50	130.24	115.30
1	A	298	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	L	554	ASP	CB-CA-C	-6.05	98.30	110.40
1	D	579	MET	CG-SD-CE	-6.05	90.52	100.20
1	F	215	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	K	549	LEU	CA-CB-CG	5.99	129.08	115.30
1	F	331	LEU	CB-CG-CD1	5.91	121.05	111.00
1	L	469	LEU	CA-CB-CG	5.88	128.81	115.30
1	P	215	ASP	CB-CG-OD1	5.87	123.58	118.30
1	P	486	LEU	CA-CB-CG	5.83	128.70	115.30
1	J	162	LEU	CA-CB-CG	5.76	128.54	115.30
1	I	185	LEU	CA-CB-CG	5.66	128.31	115.30
1	M	84	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	I	611	VAL	CB-CA-C	-5.60	100.76	111.40
1	G	486	LEU	CA-CB-CG	5.60	128.17	115.30
1	G	469	LEU	CA-CB-CG	5.59	128.17	115.30
1	G	611	VAL	CB-CA-C	-5.59	100.77	111.40
1	G	631	ASP	CB-CG-OD1	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	185	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	86	GLY	N-CA-C	5.55	126.97	113.10
1	D	308	LEU	CB-CG-CD1	5.55	120.43	111.00
1	C	486	LEU	CA-CB-CG	5.52	128.00	115.30
1	H	241	GLU	CA-C-N	5.52	129.34	117.20
1	E	145	GLU	C-N-CA	5.47	135.37	121.70
1	N	629	LEU	CA-CB-CG	5.44	127.81	115.30
1	J	298	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	M	84	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	549	LEU	CA-CB-CG	5.42	127.75	115.30
1	D	162	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	208	SER	CB-CA-C	-5.40	99.84	110.10
1	K	215	ASP	CB-CG-OD1	5.37	123.14	118.30
1	L	486	LEU	CB-CG-CD2	5.34	120.08	111.00
1	F	611	VAL	CB-CA-C	-5.32	101.29	111.40
1	D	618	LEU	CB-CG-CD1	5.31	120.03	111.00
1	J	274	ASP	CB-CG-OD1	5.31	123.08	118.30
1	K	411	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	70	ASP	CB-CG-OD1	5.29	123.06	118.30
1	L	331	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	298	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	47	LEU	CA-CB-CG	5.26	127.41	115.30
1	D	478	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	C	331	LEU	CA-CB-CG	5.26	127.40	115.30
1	O	327	ASP	CB-CG-OD1	5.24	123.01	118.30
1	G	207	CYS	N-CA-C	-5.22	96.90	111.00
1	N	579	MET	CG-SD-CE	-5.20	91.88	100.20
1	J	308	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	249	ASP	CB-CG-OD2	5.17	122.95	118.30
1	K	411	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	F	215	ASP	CB-CG-OD1	5.15	122.93	118.30
1	L	476	GLU	CB-CA-C	-5.13	100.13	110.40
1	J	387	GLY	N-CA-C	-5.13	100.28	113.10
1	F	272	ASP	CB-CG-OD1	5.11	122.90	118.30
1	I	465	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	375	ASP	CB-CG-OD2	5.05	122.85	118.30
1	M	618	LEU	CA-CB-CG	5.05	126.91	115.30
1	P	145	GLU	C-N-CA	5.02	134.25	121.70
1	P	162	LEU	CA-CB-CG	5.01	126.83	115.30
1	O	162	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLU	Peptide
1	E	282	PHE	Peptide
1	E	316	MET	Peptide
1	H	282	PHE	Peptide
1	J	291	ASN	Peptide
1	J	597	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5106	0	4989	129	0
1	B	5084	0	4967	174	0
1	C	5091	0	4976	158	1
1	D	5078	0	4962	138	1
1	E	5069	0	4953	160	0
1	F	5084	0	4967	153	0
1	G	5070	0	4955	145	0
1	H	5091	0	4976	136	0
1	I	5122	0	5007	173	0
1	J	5122	0	5007	184	0
1	K	5106	0	4989	212	0
1	L	5122	0	5007	136	0
1	M	5049	0	4935	270	0
1	N	5084	0	4967	225	1
1	O	5106	0	4989	214	0
1	P	5069	0	4953	158	1
1	Q	5039	0	4927	233	0
1	R	5084	0	4967	202	0
2	A	26	0	19	0	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	3	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	3	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
2	N	26	0	19	1	0
2	O	26	0	19	0	0
2	P	26	0	19	3	0
2	Q	26	0	19	1	0
2	R	26	0	19	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	5	0	0	0	0
4	A	105	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	1	0
4	D	93	0	0	3	0
4	E	41	0	0	0	0
4	F	12	0	0	1	0
4	G	19	0	0	1	0
4	H	59	0	0	1	0
4	I	21	0	0	3	0
4	J	12	0	0	1	0
4	K	6	0	0	0	0
4	L	85	0	0	4	0
4	M	2	0	0	2	0
4	P	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	92645	0	89835	3158	2

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 17.

All (3158) 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:L:490:PRO:HB3	1:L:569:MET:CE	1.55	1.36
1:G:490:PRO:HB3	1:G:569:MET:CE	1.58	1.32
1:F:490:PRO:HB3	1:F:569:MET:CE	1.60	1.28
1:M:569:MET:HG3	1:M:624:LEU:CD1	1.67	1.23
1:B:490:PRO:HB3	1:B:569:MET:CE	1.71	1.20
1:D:497:GLN:NE2	1:D:497:GLN:H	1.42	1.18
1:N:379:LYS:HA	1:N:399:THR:HG22	1.28	1.16
1:A:490:PRO:HB3	1:A:569:MET:CE	1.76	1.16
1:E:478:ARG:HH21	1:E:478:ARG:HG2	0.99	1.15
1:Q:375:ASP:HA	1:Q:399:THR:HG21	1.28	1.14
1:O:393:GLY:HA3	1:O:405:ILE:CD1	1.77	1.13
1:Q:153:ARG:HG3	1:Q:153:ARG:HH11	1.04	1.12
1:Q:218:LEU:H	1:Q:303:GLN:NE2	1.44	1.12
1:J:597:SER:HB2	1:J:598:ALA:HB2	1.32	1.12
1:O:627:HIS:HB2	1:O:640:GLN:HB2	1.13	1.11
1:H:490:PRO:HB3	1:H:569:MET:CE	1.81	1.11
1:L:67:HIS:CE1	1:L:91:THR:HG23	1.86	1.11
1:Q:68:VAL:HG13	1:Q:90:VAL:HG13	1.30	1.10
1:F:218:LEU:H	1:F:303:GLN:NE2	1.49	1.10
1:C:490:PRO:HB3	1:C:569:MET:CE	1.82	1.10
1:H:490:PRO:HB3	1:H:569:MET:HE2	1.30	1.10
1:J:490:PRO:HB3	1:J:569:MET:HE3	1.24	1.09
1:F:50:LEU:O	1:F:54:ILE:HD12	1.52	1.09
1:K:67:HIS:CE1	1:K:91:THR:HG22	1.85	1.09
1:L:490:PRO:HB3	1:L:569:MET:HE1	1.27	1.08
1:L:67:HIS:HE1	1:L:91:THR:HG23	0.96	1.08
1:M:280:THR:HG23	1:M:281:THR:HG22	1.35	1.08
1:I:26:GLN:HG2	1:I:30:ARG:HH12	1.12	1.08
1:C:169:VAL:HG22	1:C:241:GLU:HG2	1.14	1.08
1:J:490:PRO:HB3	1:J:569:MET:CE	1.84	1.08
1:G:169:VAL:HG12	1:G:241:GLU:HG3	1.25	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PRO:HB3	1:A:569:MET:HE2	1.36	1.08
1:Q:264:ILE:HG12	1:Q:264:ILE:O	1.44	1.07
1:R:433:LYS:HE2	1:R:433:LYS:H	1.20	1.06
1:M:569:MET:HG3	1:M:624:LEU:HD12	1.32	1.06
1:N:54:ILE:CA	1:N:58:LYS:HZ3	1.69	1.06
1:O:227:ARG:NH2	1:O:261:SER:O	1.88	1.06
1:M:91:THR:HG22	1:M:117:THR:HG23	1.32	1.05
1:K:67:HIS:HE1	1:K:91:THR:HG22	0.94	1.05
1:Q:39:ASP:OD2	1:Q:298:ARG:HD3	1.56	1.05
1:C:168:ARG:HG2	1:C:168:ARG:HH11	0.90	1.05
1:H:273:ILE:HG13	1:H:275:MET:HE3	1.39	1.04
1:G:490:PRO:HB3	1:G:569:MET:HE3	1.36	1.03
1:N:55:ALA:N	1:N:58:LYS:HZ2	1.54	1.03
1:A:168:ARG:HG2	1:A:168:ARG:HH11	0.89	1.03
1:K:67:HIS:HE1	1:K:91:THR:CG2	1.69	1.03
1:Q:168:ARG:HH11	1:Q:168:ARG:HG2	1.24	1.03
1:I:51:LYS:HE2	1:I:85:GLU:OE2	1.56	1.03
1:N:269:MET:HG2	1:N:306:TYR:HE1	1.24	1.03
1:N:444:VAL:HG13	1:N:479:VAL:HB	1.40	1.03
1:M:478:ARG:HG2	1:M:478:ARG:HH21	1.20	1.03
1:A:103:ALA:O	1:A:107:THR:HB	1.57	1.02
1:N:54:ILE:HA	1:N:58:LYS:NZ	1.75	1.02
1:N:54:ILE:HA	1:N:58:LYS:HZ3	0.87	1.02
1:C:450:TYR:H	1:C:459:HIS:HD2	1.08	1.02
1:N:63:ASP:HB2	1:N:65:LYS:H	1.23	1.02
1:I:210:THR:HG21	4:I:809:HOH:O	1.60	1.02
1:D:490:PRO:HB3	1:D:569:MET:HE3	1.37	1.02
1:G:490:PRO:CB	1:G:569:MET:CE	2.38	1.01
1:H:547:GLU:OE2	1:H:550:ARG:NH1	1.92	1.01
1:I:497:GLN:HE21	1:I:497:GLN:N	1.56	1.01
1:F:490:PRO:HB3	1:F:569:MET:HE1	1.38	1.01
1:A:420:ILE:HD11	1:A:428:VAL:HG22	1.43	1.01
1:B:490:PRO:HB3	1:B:569:MET:HE1	1.42	1.00
1:C:168:ARG:HG2	1:C:168:ARG:NH1	1.72	1.00
1:I:67:HIS:HE1	1:I:91:THR:HG23	1.26	1.00
1:P:241:GLU:HG3	1:P:277:ARG:HH21	1.26	1.00
1:J:490:PRO:CB	1:J:569:MET:CE	2.39	1.00
1:Q:137:ILE:HG13	1:Q:169:VAL:HG12	1.44	1.00
1:K:68:VAL:HG22	1:K:136:ILE:HB	1.43	0.99
1:O:393:GLY:HA3	1:O:405:ILE:HD11	1.03	0.99
1:A:478:ARG:HH21	1:A:478:ARG:HG2	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ASP:OD2	1:J:298:ARG:HD3	1.61	0.98
1:H:497:GLN:H	1:H:497:GLN:NE2	1.60	0.98
1:H:478:ARG:HH21	1:H:478:ARG:HG2	1.29	0.98
1:F:490:PRO:HB3	1:F:569:MET:HE3	1.44	0.98
1:H:497:GLN:H	1:H:497:GLN:HE21	1.09	0.98
1:Q:68:VAL:HG13	1:Q:90:VAL:CG1	1.94	0.98
1:I:26:GLN:HG2	1:I:30:ARG:NH1	1.76	0.98
1:K:67:HIS:CE1	1:K:91:THR:CG2	2.47	0.97
1:R:450:TYR:H	1:R:459:HIS:CD2	1.82	0.97
1:H:480:GLU:OE2	1:H:482:HIS:HD2	1.44	0.97
1:R:556:ARG:HG3	1:R:556:ARG:HH11	1.29	0.97
1:C:169:VAL:CG2	1:C:241:GLU:HG2	1.95	0.96
1:A:67:HIS:HE1	1:A:91:THR:CG2	1.77	0.96
1:A:168:ARG:NH1	1:A:168:ARG:HG2	1.69	0.96
1:I:497:GLN:NE2	1:I:497:GLN:H	1.63	0.96
1:R:450:TYR:H	1:R:459:HIS:HD2	1.04	0.96
1:M:478:ARG:HH21	1:M:478:ARG:CG	1.79	0.96
1:E:317:ASN:HD22	1:E:317:ASN:H	0.99	0.96
1:Q:42:ARG:NH1	1:Q:140:GLU:HG2	1.80	0.96
1:J:597:SER:HB2	1:J:598:ALA:CB	1.94	0.96
1:E:67:HIS:HE1	1:E:91:THR:HG23	1.30	0.96
1:A:497:GLN:NE2	1:A:497:GLN:H	1.63	0.95
1:N:438:THR:HG21	1:O:629:LEU:HD21	1.48	0.95
1:Q:218:LEU:N	1:Q:303:GLN:HE21	1.63	0.95
1:D:280:THR:HG23	1:D:281:THR:HG22	1.46	0.95
1:N:169:VAL:HG11	1:N:240:PHE:O	1.68	0.94
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.32	0.94
1:O:73:THR:HB	1:O:92:ALA:HB1	1.49	0.94
1:A:497:GLN:HE21	1:A:497:GLN:H	1.08	0.94
1:B:39:ASP:OD2	1:B:298:ARG:HD3	1.66	0.94
1:L:577:MET:HE3	1:L:641:PHE:HZ	1.30	0.94
1:J:490:PRO:CB	1:J:569:MET:HE3	1.97	0.94
1:H:480:GLU:OE2	1:H:482:HIS:CD2	2.21	0.94
1:A:502:ASP:OD2	1:A:616:THR:HG21	1.66	0.94
1:M:450:TYR:H	1:M:459:HIS:HD2	1.01	0.94
1:F:42:ARG:NH1	1:F:140:GLU:HG2	1.83	0.94
1:E:67:HIS:CE1	1:E:91:THR:HG23	2.03	0.93
1:P:450:TYR:H	1:P:459:HIS:HD2	1.07	0.93
1:D:497:GLN:HE21	1:D:497:GLN:N	1.64	0.93
1:D:490:PRO:HB3	1:D:569:MET:CE	1.97	0.93
1:J:158:ALA:HA	1:J:162:LEU:HD23	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:ARG:HG2	1:N:168:ARG:HH11	1.34	0.93
1:N:255:GLU:HG2	1:N:321:GLU:HG2	1.51	0.92
1:C:490:PRO:HB3	1:C:569:MET:HE3	1.47	0.92
1:A:228:GLU:OE2	1:A:290:LYS:NZ	2.02	0.92
1:J:168:ARG:HG2	1:J:168:ARG:HH11	1.33	0.92
1:B:450:TYR:H	1:B:459:HIS:HD2	0.99	0.92
1:P:157:GLU:HA	1:P:160:GLU:HG3	1.51	0.92
1:E:259:HIS:HD2	1:E:260:SER:OG	1.51	0.92
1:H:87:ALA:O	1:H:115:LYS:HE3	1.67	0.92
1:A:133:ARG:HB2	1:A:164:LYS:HG3	1.51	0.92
1:I:490:PRO:HB3	1:I:569:MET:HE2	1.52	0.92
1:E:490:PRO:HB3	1:E:569:MET:CE	1.99	0.92
1:O:218:LEU:H	1:O:303:GLN:NE2	1.68	0.92
1:E:169:VAL:HG12	1:E:241:GLU:HG2	1.52	0.92
1:J:497:GLN:H	1:J:497:GLN:HE21	1.16	0.92
1:D:478:ARG:HG2	1:D:478:ARG:HH21	1.35	0.91
1:E:478:ARG:NH2	1:E:478:ARG:HG2	1.79	0.91
1:L:42:ARG:NH1	1:L:140:GLU:HG2	1.85	0.91
1:L:490:PRO:CB	1:L:569:MET:HE1	2.00	0.91
1:F:218:LEU:H	1:F:303:GLN:HE21	1.13	0.91
1:H:273:ILE:HG13	1:H:275:MET:CE	2.00	0.91
1:D:168:ARG:NH2	1:D:276:ASP:O	2.03	0.91
1:Q:180:PRO:HG2	1:Q:230:SER:HB3	1.52	0.91
1:P:478:ARG:HH21	1:P:478:ARG:HG2	1.36	0.91
1:P:490:PRO:HB3	1:P:569:MET:CE	2.00	0.91
1:E:42:ARG:NH1	1:E:140:GLU:HG2	1.84	0.91
1:H:117:THR:OG1	1:J:131:GLY:HA3	1.70	0.91
1:D:497:GLN:HE21	1:D:497:GLN:H	0.97	0.91
1:C:137:ILE:HB	1:C:169:VAL:HG12	1.50	0.91
1:D:480:GLU:OE2	1:D:482:HIS:HD2	1.54	0.91
1:G:490:PRO:CB	1:G:569:MET:HE1	2.01	0.90
1:O:39:ASP:OD2	1:O:298:ARG:HD3	1.71	0.90
1:L:168:ARG:HH11	1:L:168:ARG:HG2	1.35	0.90
1:P:42:ARG:NH1	1:P:140:GLU:HG2	1.86	0.90
1:C:168:ARG:HH11	1:C:168:ARG:CG	1.81	0.90
1:M:91:THR:HG22	1:M:117:THR:CG2	2.02	0.90
1:L:169:VAL:HG13	1:L:241:GLU:HG2	1.52	0.90
1:O:497:GLN:HE21	1:O:497:GLN:H	1.14	0.90
1:R:196:ASN:HB2	1:R:201:GLU:OE2	1.71	0.90
1:M:497:GLN:NE2	1:M:497:GLN:H	1.68	0.90
1:L:67:HIS:HE1	1:L:91:THR:CG2	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:490:PRO:HB3	1:P:569:MET:HE1	1.52	0.90
1:D:434:VAL:CG1	1:D:469:LEU:HD13	2.02	0.90
1:M:42:ARG:HH11	1:M:140:GLU:HG3	1.36	0.90
1:D:42:ARG:HH11	1:D:140:GLU:HG2	1.34	0.90
1:L:379:LYS:HA	1:L:399:THR:HG23	1.53	0.90
1:I:450:TYR:H	1:I:459:HIS:HD2	1.12	0.89
1:K:123:SER:HB3	2:K:701:SAH:HN62	1.34	0.89
1:M:178:ILE:O	1:M:233:ILE:HG22	1.72	0.89
1:G:379:LYS:HA	1:G:399:THR:HG23	1.55	0.89
1:E:379:LYS:HA	1:E:399:THR:CG2	2.03	0.89
1:C:314:VAL:HG21	1:C:320:PHE:CD2	2.06	0.89
1:A:168:ARG:CG	1:A:168:ARG:HH11	1.81	0.89
1:A:67:HIS:HE1	1:A:91:THR:HG22	1.37	0.89
1:P:42:ARG:HH11	1:P:140:GLU:HG2	1.36	0.89
1:I:379:LYS:HA	1:I:399:THR:HG23	1.53	0.89
1:J:370:PHE:O	1:J:374:VAL:HG23	1.72	0.89
1:A:434:VAL:CG1	1:A:469:LEU:HD13	2.03	0.88
1:N:55:ALA:N	1:N:58:LYS:NZ	2.20	0.88
1:Q:196:ASN:HB2	1:Q:201:GLU:OE2	1.72	0.88
1:O:490:PRO:HB3	1:O:569:MET:CE	2.03	0.88
1:M:450:TYR:H	1:M:459:HIS:CD2	1.89	0.88
1:I:67:HIS:CE1	1:I:91:THR:HG23	2.08	0.88
1:G:379:LYS:HA	1:G:399:THR:CG2	2.04	0.88
1:F:497:GLN:HE21	1:F:497:GLN:H	1.19	0.88
1:R:291:ASN:HB3	1:R:295:TYR:HB2	1.56	0.88
1:O:643:LYS:H	1:O:643:LYS:HD2	1.37	0.88
1:Q:153:ARG:NH1	1:Q:153:ARG:HG3	1.74	0.88
1:J:194:ARG:HG2	1:J:201:GLU:HB2	1.54	0.87
1:R:547:GLU:OE2	1:R:550:ARG:NH2	2.07	0.87
1:Q:68:VAL:CG1	1:Q:90:VAL:HG13	2.03	0.87
1:D:379:LYS:HA	1:D:399:THR:HG23	1.56	0.87
1:M:497:GLN:HE21	1:M:497:GLN:H	1.19	0.87
1:O:373:GLU:O	1:O:377:LEU:HD12	1.75	0.87
1:M:68:VAL:HG22	1:M:136:ILE:HB	1.55	0.87
1:Q:450:TYR:H	1:Q:459:HIS:HD2	1.18	0.87
1:H:450:TYR:H	1:H:459:HIS:HD2	1.22	0.87
1:A:490:PRO:CB	1:A:569:MET:HE2	2.06	0.86
1:N:147:ILE:HD11	1:N:331:LEU:HD13	1.57	0.86
1:I:570:SER:HB3	1:I:622:LYS:HG2	1.54	0.86
1:B:550:ARG:H	1:B:560:GLN:HE22	1.23	0.86
1:N:478:ARG:HG2	1:N:478:ARG:HH21	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LYS:HA	1:D:399:THR:CG2	2.06	0.86
1:E:57:LYS:O	1:E:66:VAL:HG21	1.75	0.86
1:F:379:LYS:HA	1:F:399:THR:HG22	1.57	0.86
1:K:42:ARG:NH1	1:K:140:GLU:HG2	1.89	0.86
1:P:146:LEU:H	1:P:146:LEU:HD23	1.40	0.86
1:L:490:PRO:CB	1:L:569:MET:CE	2.50	0.86
1:M:379:LYS:HA	1:M:399:THR:CG2	2.06	0.86
1:J:483:MET:HB3	1:J:582:GLU:HG3	1.55	0.86
1:M:181:VAL:HG21	1:M:268:LEU:HD11	1.57	0.86
1:O:393:GLY:CA	1:O:405:ILE:HD11	1.99	0.85
1:P:104:ARG:HB2	1:P:104:ARG:CZ	2.04	0.85
1:F:39:ASP:OD2	1:F:298:ARG:HD3	1.76	0.85
1:F:450:TYR:H	1:F:459:HIS:HD2	1.25	0.85
1:I:323:VAL:HG11	1:I:340:LYS:HD3	1.57	0.85
1:D:42:ARG:NH1	1:D:140:GLU:HG2	1.90	0.85
1:N:50:LEU:O	1:N:54:ILE:HG23	1.77	0.85
1:Q:153:ARG:CG	1:Q:153:ARG:HH11	1.89	0.85
1:L:168:ARG:NH1	1:L:241:GLU:OE2	2.08	0.85
1:F:218:LEU:HD12	1:F:303:GLN:CB	2.06	0.85
1:M:478:ARG:HG2	1:M:478:ARG:NH2	1.89	0.85
1:L:490:PRO:HB3	1:L:569:MET:HE3	1.57	0.85
1:C:450:TYR:H	1:C:459:HIS:CD2	1.94	0.85
1:N:58:LYS:HE2	1:N:66:VAL:HG21	1.57	0.85
1:M:379:LYS:HA	1:M:399:THR:HG23	1.57	0.85
1:K:569:MET:HG3	1:K:624:LEU:HD11	1.58	0.85
1:R:622:LYS:H	1:R:622:LYS:HD2	1.41	0.85
1:K:169:VAL:HG13	1:K:241:GLU:HG2	1.57	0.84
1:B:104:ARG:O	1:B:108:SER:HB3	1.77	0.84
1:F:565:ASN:HD21	1:F:644:SER:HB2	1.42	0.84
1:J:438:THR:HG21	1:K:629:LEU:HD21	1.59	0.84
1:O:528:ILE:H	1:O:528:ILE:HD12	1.41	0.84
1:B:163:ALA:HB1	1:B:167:CYS:SG	2.17	0.84
1:D:434:VAL:HG12	1:D:469:LEU:HD13	1.60	0.84
1:G:497:GLN:HE21	1:G:497:GLN:H	1.25	0.84
1:O:373:GLU:HG3	1:O:377:LEU:HD11	1.59	0.83
1:P:450:TYR:H	1:P:459:HIS:CD2	1.94	0.83
1:F:553:ILE:HG22	1:F:553:ILE:O	1.77	0.83
1:B:490:PRO:CB	1:B:569:MET:HE1	2.08	0.83
1:R:51:LYS:HZ2	1:R:51:LYS:HB2	1.43	0.83
1:E:87:ALA:O	1:E:115:LYS:HE2	1.78	0.83
1:F:275:MET:HE1	1:F:283:ILE:HG13	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:PRO:CB	1:D:569:MET:CE	2.56	0.83
1:A:67:HIS:CE1	1:A:91:THR:CG2	2.62	0.83
1:R:66:VAL:HA	1:R:135:ASP:OD2	1.76	0.83
1:O:233:ILE:HD11	1:O:254:ARG:CB	2.08	0.83
1:F:150:GLY:O	1:F:154:THR:OG1	1.96	0.83
1:N:379:LYS:HA	1:N:399:THR:CG2	2.08	0.83
1:N:480:GLU:OE2	1:N:482:HIS:HD2	1.60	0.83
1:R:379:LYS:HA	1:R:399:THR:CG2	2.08	0.83
1:Q:378:SER:HB2	1:Q:399:THR:HG23	1.60	0.82
1:K:550:ARG:H	1:K:560:GLN:HE22	1.24	0.82
1:N:254:ARG:O	1:N:321:GLU:HA	1.79	0.82
1:N:27:GLU:OE2	1:N:96:PHE:CE1	2.32	0.82
1:B:450:TYR:H	1:B:459:HIS:CD2	1.91	0.82
1:Q:254:ARG:O	1:Q:321:GLU:HA	1.79	0.82
1:M:110:SER:HB2	1:M:111:PRO:HD2	1.62	0.82
1:O:450:TYR:H	1:O:459:HIS:HD2	1.27	0.82
1:G:66:VAL:HG12	1:G:87:ALA:HA	1.62	0.82
1:L:631:ASP:OD1	1:L:633:SER:HB2	1.80	0.82
1:K:388:GLU:OE1	1:K:452:SER:HB2	1.79	0.82
1:K:379:LYS:HA	1:K:399:THR:HG23	1.60	0.82
1:L:577:MET:CE	1:L:641:PHE:HZ	1.92	0.82
1:A:506:VAL:HG12	1:A:507:ASN:HD22	1.45	0.82
1:P:104:ARG:O	1:P:108:SER:HB2	1.80	0.81
1:J:189:PHE:CD1	1:J:359:TYR:HB2	2.14	0.81
1:N:63:ASP:CB	1:N:65:LYS:H	1.93	0.81
1:K:42:ARG:HH12	1:K:140:GLU:HG2	1.45	0.81
1:F:553:ILE:O	1:F:553:ILE:CG2	2.29	0.81
1:B:490:PRO:HB3	1:B:569:MET:HE3	1.59	0.81
1:C:314:VAL:CG2	1:C:320:PHE:CD2	2.63	0.81
1:Q:478:ARG:HG2	1:Q:478:ARG:HH21	1.45	0.81
1:Q:183:SER:H	1:Q:265:ASP:HB2	1.46	0.81
1:H:42:ARG:HH11	1:H:140:GLU:HG2	1.46	0.81
1:J:243:GLU:OE1	1:J:243:GLU:N	2.12	0.81
1:P:259:HIS:HD2	1:P:260:SER:OG	1.62	0.81
1:G:169:VAL:CG1	1:G:241:GLU:HG3	2.09	0.81
1:C:480:GLU:OE2	1:C:482:HIS:HD2	1.64	0.81
1:N:269:MET:HG2	1:N:306:TYR:CE1	2.13	0.81
1:J:497:GLN:H	1:J:497:GLN:NE2	1.78	0.81
1:M:50:LEU:HD23	1:M:170:VAL:HG21	1.62	0.81
1:R:556:ARG:CG	1:R:556:ARG:HH11	1.93	0.81
1:E:379:LYS:HA	1:E:399:THR:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:444:VAL:HG13	1:M:479:VAL:HB	1.61	0.80
1:B:216:VAL:O	1:B:302:MET:HG2	1.81	0.80
1:D:450:TYR:H	1:D:459:HIS:HD2	1.27	0.80
1:Q:216:VAL:O	1:Q:302:MET:HG2	1.81	0.80
1:Q:264:ILE:HD11	1:Q:267:LEU:HD21	1.63	0.80
1:M:95:VAL:CG2	1:M:122:ARG:HG3	2.11	0.80
1:P:379:LYS:HA	1:P:399:THR:HG23	1.63	0.80
1:E:478:ARG:HH21	1:E:478:ARG:CG	1.90	0.80
1:Q:264:ILE:CG1	1:Q:264:ILE:O	2.29	0.80
1:E:258:ALA:HB3	1:E:315:GLU:O	1.82	0.79
1:E:317:ASN:H	1:E:317:ASN:ND2	1.79	0.79
1:R:379:LYS:HA	1:R:399:THR:HG21	1.64	0.79
1:R:567:ASP:HA	1:R:623:SER:HB2	1.64	0.79
1:B:140:GLU:O	1:B:140:GLU:HG3	1.82	0.79
1:M:39:ASP:OD2	1:M:298:ARG:HD2	1.81	0.79
1:J:450:TYR:H	1:J:459:HIS:HD2	1.31	0.79
1:J:596:SER:O	1:J:599:GLY:N	2.11	0.79
1:I:169:VAL:HG13	1:I:241:GLU:HG2	1.65	0.79
1:P:5:LYS:HA	1:R:420:ILE:HD11	1.65	0.79
1:F:50:LEU:O	1:F:54:ILE:CD1	2.31	0.79
1:D:169:VAL:HG13	1:D:241:GLU:HG2	1.63	0.79
1:B:39:ASP:O	1:B:43:ASN:ND2	2.16	0.79
1:L:210:THR:HB	4:L:815:HOH:O	1.83	0.79
1:K:141:VAL:HG13	1:K:141:VAL:O	1.81	0.79
1:N:242:HIS:HB3	1:N:245:LYS:HD3	1.64	0.79
1:M:132:SER:N	1:P:104:ARG:NH2	2.31	0.79
1:G:158:ALA:HA	1:G:162:LEU:HD23	1.64	0.79
1:M:569:MET:CG	1:M:624:LEU:CD1	2.58	0.78
1:Q:168:ARG:CG	1:Q:168:ARG:HH11	1.96	0.78
1:J:239:ASP:OD2	1:J:242:HIS:HD2	1.66	0.78
1:Q:218:LEU:N	1:Q:303:GLN:NE2	2.25	0.78
1:A:169:VAL:HG13	1:A:241:GLU:HG2	1.63	0.78
1:O:233:ILE:HD11	1:O:254:ARG:HB3	1.65	0.78
1:M:41:ASP:O	1:M:45:LYS:HB2	1.83	0.78
1:M:480:GLU:OE2	1:M:482:HIS:HD2	1.67	0.78
1:G:497:GLN:NE2	1:G:497:GLN:H	1.82	0.78
1:R:73:THR:OG1	1:R:76:GLY:HA2	1.83	0.78
1:O:42:ARG:NH1	1:O:140:GLU:HG2	1.98	0.78
1:K:76:GLY:O	1:K:79:SER:N	2.17	0.78
1:K:450:TYR:H	1:K:459:HIS:HD2	1.30	0.78
1:G:450:TYR:H	1:G:459:HIS:HD2	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ASN:HD22	1:E:317:ASN:N	1.75	0.78
1:L:42:ARG:HH11	1:L:140:GLU:HG2	1.48	0.78
1:N:142:PHE:CD1	1:N:146:LEU:HD12	2.20	0.77
1:K:541:VAL:HG23	1:K:601:PRO:HG3	1.66	0.77
1:Q:178:ILE:HD13	1:Q:235:ALA:HB2	1.65	0.77
1:N:133:ARG:HB3	1:N:133:ARG:HH21	1.48	0.77
1:Q:232:PRO:HG2	1:Q:290:LYS:HE2	1.65	0.77
1:F:450:TYR:H	1:F:459:HIS:CD2	2.02	0.77
1:N:67:HIS:H	1:N:135:ASP:HB2	1.49	0.77
1:J:480:GLU:OE2	1:J:482:HIS:HD2	1.66	0.77
1:C:490:PRO:CB	1:C:569:MET:CE	2.63	0.77
1:M:280:THR:HG23	1:M:281:THR:CG2	2.14	0.77
1:Q:247:ILE:HG12	1:Q:250:GLU:OE2	1.84	0.77
1:D:67:HIS:HE1	1:D:91:THR:CG2	1.96	0.77
1:J:383:VAL:HG21	1:J:445:LEU:HD22	1.67	0.77
1:B:243:GLU:N	1:B:243:GLU:OE1	2.13	0.77
1:Q:218:LEU:H	1:Q:303:GLN:HE21	0.78	0.77
1:G:103:ALA:O	1:G:107:THR:HG23	1.84	0.77
1:E:434:VAL:CG1	1:E:469:LEU:HD13	2.15	0.77
1:B:179:VAL:HG12	1:B:180:PRO:O	1.85	0.77
1:F:104:ARG:O	1:F:108:SER:HB3	1.84	0.77
1:G:95:VAL:HG22	1:G:95:VAL:O	1.85	0.77
1:A:450:TYR:H	1:A:459:HIS:HD2	1.33	0.77
1:N:530:ASP:OD1	1:N:531:GLU:N	2.17	0.77
1:B:42:ARG:NH1	1:B:140:GLU:HG2	2.00	0.76
1:F:206:ARG:HH12	1:F:310:GLU:HG3	1.50	0.76
1:N:566:ILE:HG22	1:N:569:MET:CE	2.15	0.76
1:H:450:TYR:H	1:H:459:HIS:CD2	2.04	0.76
1:C:489:ILE:O	1:C:576:PRO:HD2	1.86	0.76
1:B:269:MET:HG2	1:B:306:TYR:HE2	1.50	0.76
1:R:450:TYR:N	1:R:459:HIS:HD2	1.80	0.76
1:O:411:ARG:O	1:O:415:ILE:HD12	1.84	0.76
1:A:67:HIS:CE1	1:A:91:THR:HG22	2.20	0.76
1:I:141:VAL:O	1:I:141:VAL:HG12	1.85	0.76
1:R:478:ARG:HH21	1:R:478:ARG:HG2	1.50	0.76
1:L:467:GLU:HG3	1:L:555:GLY:O	1.86	0.76
1:D:80:LEU:HB3	1:D:509:PHE:CE1	2.19	0.76
1:M:278:ASN:O	1:M:280:THR:HG22	1.85	0.76
1:D:291:ASN:H	1:D:292:LYS:NZ	1.84	0.76
1:I:273:ILE:HD12	1:I:275:MET:HE1	1.67	0.76
1:H:497:GLN:N	1:H:497:GLN:HE21	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:ARG:NH2	1:I:261:SER:O	2.19	0.75
1:M:222:LYS:O	1:M:225:GLU:HG2	1.86	0.75
1:K:480:GLU:OE2	1:K:482:HIS:HD2	1.67	0.75
1:F:218:LEU:HD12	1:F:303:GLN:HB3	1.67	0.75
1:Q:232:PRO:CG	1:Q:290:LYS:HE2	2.17	0.75
1:C:4:GLU:OE2	1:C:13:ARG:HD3	1.86	0.75
1:N:566:ILE:CG2	1:N:569:MET:HE3	2.16	0.75
1:Q:276:ASP:O	1:Q:277:ARG:HB2	1.87	0.75
1:M:412:PHE:HE2	1:M:451:MET:HG2	1.51	0.75
1:I:568:ASN:O	1:I:572:SER:OG	2.03	0.75
1:Q:480:GLU:HG3	1:Q:584:GLY:H	1.52	0.75
1:I:434:VAL:HG12	1:I:469:LEU:HD13	1.69	0.75
1:H:478:ARG:HH21	1:H:478:ARG:CG	2.00	0.75
1:O:490:PRO:HB3	1:O:569:MET:HE3	1.69	0.75
1:C:42:ARG:NH1	1:C:140:GLU:HG2	2.02	0.75
1:C:616:THR:O	1:C:619:ARG:HG2	1.85	0.75
1:O:442:ASP:O	1:O:478:ARG:HB2	1.87	0.75
1:J:168:ARG:HG2	1:J:168:ARG:NH1	2.02	0.75
1:I:275:MET:HA	1:I:275:MET:HE2	1.69	0.75
1:N:450:TYR:H	1:N:459:HIS:HD2	1.34	0.75
1:M:553:ILE:HG13	1:M:553:ILE:O	1.84	0.74
1:E:42:ARG:HH12	1:E:140:GLU:HG2	1.49	0.74
1:E:450:TYR:H	1:E:459:HIS:HD2	1.32	0.74
1:M:615:ILE:O	1:M:617:ALA:N	2.20	0.74
1:B:169:VAL:HG13	1:B:241:GLU:HG2	1.70	0.74
1:M:5:LYS:HA	1:O:420:ILE:HD11	1.69	0.74
1:F:275:MET:CE	1:F:283:ILE:HG13	2.16	0.74
1:C:4:GLU:OE2	1:C:13:ARG:CD	2.36	0.74
1:E:497:GLN:NE2	1:E:497:GLN:H	1.84	0.74
1:F:497:GLN:NE2	1:F:497:GLN:H	1.86	0.74
1:O:566:ILE:O	1:O:623:SER:HA	1.85	0.74
1:M:95:VAL:HG21	1:M:122:ARG:HG3	1.69	0.74
1:O:169:VAL:HG13	1:O:241:GLU:HG2	1.68	0.74
1:N:150:GLY:O	1:N:154:THR:OG1	2.06	0.74
1:R:371:LYS:O	1:R:375:ASP:OD1	2.06	0.74
1:M:480:GLU:OE2	1:M:482:HIS:CD2	2.41	0.74
1:D:67:HIS:HE1	1:D:91:THR:HG23	1.49	0.74
1:C:67:HIS:HE1	1:C:91:THR:HG22	1.53	0.74
1:O:4:GLU:OE2	1:O:13:ARG:HD3	1.88	0.74
1:R:51:LYS:HB2	1:R:51:LYS:NZ	2.02	0.73
1:H:66:VAL:N	1:H:88:ASP:OD2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:384:ALA:HB3	1:R:444:VAL:HG12	1.70	0.73
1:Q:590:THR:O	1:Q:609:GLN:NE2	2.20	0.73
1:M:450:TYR:N	1:M:459:HIS:HD2	1.81	0.73
1:O:382:HIS:CD2	1:O:441:PRO:HA	2.23	0.73
1:K:271:TRP:O	1:K:285:MET:HB2	1.88	0.73
1:B:314:VAL:HG22	1:B:315:GLU:H	1.53	0.73
1:N:566:ILE:HG21	1:N:569:MET:HE3	1.71	0.73
1:J:36:MET:HA	1:J:300:HIS:CD2	2.22	0.73
1:O:643:LYS:CD	1:O:643:LYS:H	1.99	0.73
1:L:273:ILE:HG13	1:L:275:MET:HE3	1.68	0.73
1:N:104:ARG:O	1:N:108:SER:OG	2.04	0.73
1:O:627:HIS:CB	1:O:640:GLN:HB2	2.08	0.73
1:K:550:ARG:N	1:K:560:GLN:HE22	1.87	0.73
1:L:103:ALA:O	1:L:107:THR:HB	1.89	0.73
1:Q:222:LYS:HB2	1:Q:225:GLU:HG2	1.71	0.73
1:L:378:SER:HB2	1:L:399:THR:HG22	1.71	0.73
1:K:73:THR:OG1	1:K:76:GLY:HA2	1.89	0.72
1:I:278:ASN:O	1:I:280:THR:HG23	1.89	0.72
1:H:490:PRO:CB	1:H:569:MET:CE	2.64	0.72
1:H:42:ARG:NH1	1:H:140:GLU:HG2	2.04	0.72
1:N:81:MET:O	1:N:84:ARG:O	2.07	0.72
1:M:42:ARG:NH1	1:M:140:GLU:HG3	2.04	0.72
1:B:392:LEU:O	1:B:392:LEU:HD23	1.89	0.72
1:B:218:LEU:H	1:B:303:GLN:NE2	1.87	0.72
1:M:245:LYS:HE3	1:R:337:GLY:HA2	1.70	0.72
1:N:87:ALA:HA	1:N:88:ASP:HB2	1.69	0.72
1:B:43:ASN:H	1:B:43:ASN:HD22	1.38	0.72
1:M:412:PHE:CE2	1:M:451:MET:HG2	2.24	0.72
1:O:497:GLN:NE2	1:O:497:GLN:H	1.87	0.72
1:D:39:ASP:OD2	1:D:298:ARG:HD3	1.88	0.72
1:P:365:PHE:O	1:P:371:LYS:CE	2.37	0.72
1:M:126:VAL:H	1:M:161:ARG:NH2	1.86	0.72
1:O:190:ASN:HD21	1:O:209:GLY:HA3	1.53	0.72
1:H:549:LEU:HD23	1:H:637:ILE:HD13	1.70	0.72
1:E:146:LEU:HB3	1:E:271:TRP:CD1	2.25	0.72
1:A:478:ARG:HH21	1:A:478:ARG:CG	2.03	0.72
1:Q:570:SER:HB2	1:Q:622:LYS:HD3	1.72	0.72
1:I:434:VAL:CG1	1:I:469:LEU:HD13	2.20	0.72
1:N:39:ASP:OD2	1:N:298:ARG:CD	2.38	0.72
1:E:41:ASP:OD1	1:E:41:ASP:C	2.27	0.72
1:L:497:GLN:H	1:L:497:GLN:HE21	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:450:TYR:H	1:Q:459:HIS:CD2	2.07	0.71
1:I:171:PRO:HB3	1:I:275:MET:HE2	1.70	0.71
1:F:203:PRO:HA	1:F:422:TYR:CD2	2.25	0.71
1:H:169:VAL:HG12	1:H:241:GLU:HG2	1.70	0.71
1:F:244:GLU:OE1	1:F:245:LYS:HG3	1.90	0.71
1:R:176:VAL:CG1	1:R:236:PHE:HB2	2.21	0.71
1:F:616:THR:O	1:F:619:ARG:NH1	2.21	0.71
1:P:57:LYS:HE2	1:P:135:ASP:HB3	1.71	0.71
1:E:259:HIS:CD2	1:E:260:SER:OG	2.41	0.71
1:P:478:ARG:HH21	1:P:478:ARG:CG	2.03	0.71
1:P:317:ASN:O	1:P:317:ASN:ND2	2.22	0.71
1:Q:367:ASN:OD1	1:Q:370:PHE:HB2	1.90	0.71
1:F:94:GLU:OE1	2:F:701:SAH:O2'	2.08	0.71
1:M:91:THR:CG2	1:M:117:THR:HG23	2.14	0.71
1:N:133:ARG:HG3	1:N:164:LYS:HG3	1.73	0.71
1:E:550:ARG:H	1:E:560:GLN:HE22	1.37	0.71
1:I:450:TYR:H	1:I:459:HIS:CD2	2.03	0.71
1:M:45:LYS:O	1:M:275:MET:HG2	1.89	0.71
1:C:244:GLU:OE2	1:C:244:GLU:HA	1.91	0.71
1:M:145:GLU:HG3	1:M:331:LEU:HD13	1.72	0.71
1:B:145:GLU:HG2	1:B:331:LEU:HD22	1.73	0.71
1:Q:217:GLN:NE2	1:Q:298:ARG:O	2.14	0.71
1:I:443:ILE:HG12	1:I:445:LEU:HD13	1.73	0.71
1:N:55:ALA:HA	1:N:58:LYS:HD2	1.73	0.71
1:Q:169:VAL:HG21	1:Q:240:PHE:HB2	1.73	0.71
1:J:173:THR:HG22	1:J:274:ASP:HB3	1.71	0.70
1:N:566:ILE:HG22	1:N:569:MET:HE2	1.70	0.70
1:K:412:PHE:HE2	1:K:451:MET:HG2	1.56	0.70
1:K:547:GLU:OE2	1:K:550:ARG:NH1	2.20	0.70
1:K:420:ILE:HD11	1:K:428:VAL:HG22	1.72	0.70
1:E:595:ILE:CG2	1:E:599:GLY:HA2	2.21	0.70
1:A:490:PRO:HB3	1:A:569:MET:HE1	1.71	0.70
1:M:489:ILE:O	1:M:576:PRO:HD2	1.91	0.70
1:B:497:GLN:H	1:B:497:GLN:HE21	1.39	0.70
1:B:241:GLU:HB2	1:B:277:ARG:HH21	1.56	0.70
1:K:138:VAL:HG23	1:K:170:VAL:HB	1.71	0.70
1:R:291:ASN:C	1:R:292:LYS:HD2	2.12	0.70
1:M:321:GLU:O	1:M:322:ILE:HD12	1.90	0.70
1:B:450:TYR:N	1:B:459:HIS:HD2	1.82	0.70
1:R:489:ILE:O	1:R:576:PRO:HD2	1.91	0.70
1:I:490:PRO:HB3	1:I:569:MET:CE	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:273:ILE:HG13	1:L:275:MET:CE	2.22	0.70
1:K:460:LEU:HB3	1:K:463:LEU:HD23	1.72	0.70
1:P:269:MET:HG2	1:P:306:TYR:HE1	1.55	0.70
1:N:88:ASP:O	1:N:89:LYS:HG3	1.92	0.70
1:B:168:ARG:NH1	1:B:241:GLU:OE2	2.24	0.70
1:G:39:ASP:OD2	1:G:298:ARG:HD3	1.91	0.70
1:B:66:VAL:HG12	1:B:67:HIS:N	2.07	0.70
1:R:269:MET:HG2	1:R:306:TYR:HE1	1.57	0.70
1:C:95:VAL:HG21	1:C:122:ARG:HG3	1.72	0.70
1:B:227:ARG:NH2	1:B:261:SER:O	2.25	0.70
1:E:84:ARG:NH1	1:E:509:PHE:CZ	2.60	0.69
1:G:22:TYR:CE2	1:G:26:GLN:OE1	2.45	0.69
1:D:480:GLU:OE2	1:D:482:HIS:CD2	2.41	0.69
1:R:349:LEU:HD12	1:R:415:ILE:HD13	1.74	0.69
1:I:73:THR:OG1	1:I:76:GLY:HA2	1.92	0.69
1:K:169:VAL:HG13	1:K:241:GLU:CG	2.21	0.69
1:O:233:ILE:HD11	1:O:254:ARG:HB2	1.74	0.69
1:H:169:VAL:CG1	1:H:241:GLU:HG2	2.22	0.69
1:G:547:GLU:OE2	1:G:550:ARG:NH2	2.24	0.69
1:I:550:ARG:H	1:I:560:GLN:HE22	1.38	0.69
1:A:420:ILE:CD1	1:A:428:VAL:HG22	2.21	0.69
1:F:206:ARG:HH12	1:F:310:GLU:CG	2.06	0.69
1:B:497:GLN:H	1:B:497:GLN:NE2	1.90	0.69
1:J:193:PRO:HA	1:J:362:ASN:HD21	1.57	0.69
1:D:145:GLU:HA	1:D:269:MET:HE1	1.74	0.69
1:B:73:THR:HG22	1:B:94:GLU:HB2	1.72	0.69
1:K:516:GLU:O	1:K:520:LYS:HG3	1.91	0.69
1:P:278:ASN:HB2	1:P:280:THR:HG22	1.74	0.69
1:N:169:VAL:CG1	1:N:241:GLU:HG2	2.22	0.69
1:J:67:HIS:HE1	1:J:91:THR:HG22	1.57	0.69
1:H:269:MET:HG2	1:H:306:TYR:CE1	2.28	0.69
1:P:210:THR:HG21	4:P:810:HOH:O	1.93	0.69
1:K:497:GLN:NE2	1:K:573:ASN:ND2	2.40	0.69
1:G:27:GLU:HG2	1:G:96:PHE:CE1	2.26	0.69
1:B:447:GLU:N	1:B:448:PRO:HA	2.08	0.69
1:Q:42:ARG:HH12	1:Q:140:GLU:HG2	1.58	0.69
1:E:450:TYR:H	1:E:459:HIS:CD2	2.09	0.69
1:N:87:ALA:CA	1:N:88:ASP:HB2	2.22	0.69
1:I:210:THR:HB	4:I:807:HOH:O	1.92	0.69
1:P:490:PRO:CB	1:P:569:MET:HE1	2.22	0.69
1:M:51:LYS:HG2	1:M:85:GLU:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HG2	1:A:306:TYR:HE1	1.58	0.69
1:P:227:ARG:NH1	1:P:229:LEU:HD21	2.08	0.69
1:L:67:HIS:CE1	1:L:91:THR:CG2	2.66	0.69
1:N:27:GLU:OE2	1:N:96:PHE:CD1	2.45	0.69
1:D:67:HIS:CE1	1:D:91:THR:HG23	2.28	0.69
1:M:37:ILE:HG21	1:M:503:VAL:CG1	2.23	0.69
1:H:51:LYS:CG	1:H:85:GLU:HG3	2.23	0.69
1:A:434:VAL:HG12	1:A:469:LEU:HD13	1.74	0.69
1:N:566:ILE:CG2	1:N:569:MET:CE	2.70	0.69
1:C:39:ASP:OD2	1:C:298:ARG:HD3	1.93	0.69
1:C:140:GLU:HG3	1:C:140:GLU:O	1.92	0.68
1:Q:643:LYS:O	1:Q:644:SER:HB3	1.93	0.68
1:G:412:PHE:HE2	1:G:451:MET:HG2	1.58	0.68
1:B:412:PHE:HE2	1:B:451:MET:HG2	1.58	0.68
1:O:567:ASP:O	1:O:568:ASN:HB2	1.93	0.68
1:B:42:ARG:HH11	1:B:140:GLU:HG2	1.58	0.68
1:B:169:VAL:CG1	1:B:241:GLU:HG2	2.24	0.68
1:H:269:MET:HG2	1:H:306:TYR:HE1	1.58	0.68
1:A:141:VAL:O	1:A:141:VAL:HG13	1.92	0.68
2:M:701:SAH:HB1	2:M:701:SAH:H4'	1.76	0.68
1:R:433:LYS:CE	1:R:433:LYS:H	2.03	0.68
1:M:145:GLU:CG	1:M:331:LEU:HD13	2.24	0.68
1:P:190:ASN:HD21	1:P:209:GLY:HA3	1.59	0.68
1:K:580:GLU:HG2	1:K:589:SER:HB2	1.76	0.68
1:K:84:ARG:O	1:K:85:GLU:HB2	1.93	0.68
1:R:433:LYS:N	1:R:433:LYS:HE2	2.02	0.68
1:D:222:LYS:O	1:D:225:GLU:HB2	1.93	0.68
1:J:597:SER:CB	1:J:598:ALA:HB2	2.19	0.68
1:N:315:GLU:HB2	1:N:318:GLN:HG2	1.75	0.68
1:M:569:MET:HG3	1:M:624:LEU:HD11	1.74	0.68
1:A:39:ASP:OD2	1:A:298:ARG:HD3	1.93	0.68
1:J:480:GLU:OE2	1:J:482:HIS:CD2	2.46	0.68
1:Q:480:GLU:OE2	1:Q:482:HIS:HD2	1.77	0.68
1:J:42:ARG:NH1	1:J:140:GLU:HG2	2.09	0.68
1:L:280:THR:HG23	1:L:281:THR:HG22	1.74	0.68
1:P:42:ARG:HH21	1:P:43:ASN:HD21	1.41	0.68
1:D:502:ASP:OD2	1:D:616:THR:HG21	1.94	0.68
1:Q:264:ILE:HD11	1:Q:267:LEU:CD2	2.23	0.67
1:I:210:THR:CG2	4:I:809:HOH:O	2.29	0.67
1:D:490:PRO:CB	1:D:569:MET:HE3	2.17	0.67
1:N:147:ILE:HD11	1:N:331:LEU:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:LYS:HE3	1:K:65:LYS:HA	1.76	0.67
1:M:522:ARG:O	1:M:526:ASP:HB2	1.94	0.67
1:I:177:TYR:O	1:I:269:MET:HA	1.93	0.67
1:A:497:GLN:N	1:A:497:GLN:HE21	1.87	0.67
1:Q:137:ILE:CG1	1:Q:169:VAL:HG12	2.22	0.67
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.59	0.67
1:H:244:GLU:H	1:H:244:GLU:CD	1.97	0.67
1:I:173:THR:HG22	1:I:274:ASP:HB3	1.76	0.67
1:Q:190:ASN:HD21	1:Q:209:GLY:HA3	1.59	0.67
1:B:175:ASN:HD22	1:B:237:LYS:HG2	1.58	0.67
1:D:291:ASN:H	1:D:292:LYS:HZ3	1.41	0.67
1:C:95:VAL:CG2	1:C:122:ARG:HG3	2.25	0.67
1:A:480:GLU:CG	1:A:584:GLY:H	2.08	0.67
1:M:258:ALA:HB2	1:M:314:VAL:HG13	1.77	0.67
1:D:522:ARG:O	1:D:526:ASP:HB2	1.95	0.67
1:D:497:GLN:NE2	1:D:497:GLN:N	2.25	0.67
1:N:63:ASP:HB2	1:N:65:LYS:N	2.05	0.67
1:H:478:ARG:HG2	1:H:478:ARG:NH2	2.04	0.67
1:C:618:LEU:HD23	1:C:624:LEU:HD22	1.75	0.67
1:P:152:LEU:HD22	1:P:246:ILE:HG23	1.76	0.67
1:M:214:PHE:CD2	1:M:305:VAL:HG22	2.30	0.67
1:D:550:ARG:H	1:D:560:GLN:HE22	1.43	0.67
1:O:506:VAL:O	1:O:509:PHE:HB2	1.95	0.67
1:G:169:VAL:HG12	1:G:241:GLU:CG	2.16	0.67
1:E:565:ASN:HA	1:E:624:LEU:O	1.93	0.67
1:M:490:PRO:HB3	1:M:569:MET:CE	2.25	0.67
1:F:42:ARG:HH11	1:F:140:GLU:HG2	1.57	0.67
1:D:42:ARG:NH1	1:D:140:GLU:CG	2.58	0.67
1:N:497:GLN:HE21	1:N:497:GLN:H	1.41	0.67
1:I:104:ARG:HG3	1:I:118:VAL:HB	1.76	0.67
1:Q:480:GLU:OE2	1:Q:482:HIS:CD2	2.48	0.66
1:R:384:ALA:HB2	1:R:437:LEU:HD11	1.76	0.66
1:O:444:VAL:HG13	1:O:479:VAL:HA	1.76	0.66
1:R:218:LEU:H	1:R:303:GLN:HE21	1.43	0.66
1:F:141:VAL:O	1:F:141:VAL:HG12	1.94	0.66
1:J:218:LEU:H	1:J:303:GLN:HE21	1.43	0.66
1:N:137:ILE:HD11	1:N:163:ALA:HB2	1.77	0.66
1:N:163:ALA:HB1	1:N:167:CYS:SG	2.35	0.66
1:E:169:VAL:CG1	1:E:241:GLU:HG2	2.24	0.66
1:A:434:VAL:CG1	1:A:469:LEU:CD1	2.73	0.66
1:R:50:LEU:O	1:R:54:ILE:HB	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ARG:HH21	1:G:43:ASN:ND2	1.93	0.66
1:J:490:PRO:HB2	1:J:569:MET:CE	2.26	0.66
1:N:497:GLN:H	1:N:497:GLN:NE2	1.93	0.66
1:C:141:VAL:HG12	1:C:141:VAL:O	1.94	0.66
1:D:489:ILE:HG13	1:D:490:PRO:HD2	1.78	0.66
1:N:478:ARG:HH21	1:N:478:ARG:CG	2.09	0.66
1:J:239:ASP:OD2	1:J:242:HIS:CD2	2.49	0.66
1:G:478:ARG:HG3	1:G:478:ARG:HH21	1.60	0.66
1:Q:191:ASP:OD2	1:Q:194:ARG:NH1	2.29	0.66
1:R:460:LEU:HD11	1:R:637:ILE:HD11	1.78	0.66
1:P:506:VAL:HG23	1:P:511:LEU:HD12	1.78	0.66
1:Q:91:THR:HG22	1:Q:117:THR:HG23	1.77	0.66
1:E:318:GLN:OE1	1:H:368:GLN:HG2	1.96	0.66
1:I:414:ASP:O	1:I:418:LYS:HG3	1.96	0.66
1:G:490:PRO:HB3	1:G:569:MET:HE2	1.72	0.66
1:F:490:PRO:CB	1:F:569:MET:HE1	2.19	0.66
1:J:490:PRO:CB	1:J:569:MET:HE2	2.26	0.66
1:D:193:PRO:HA	1:D:362:ASN:HD21	1.61	0.66
1:Q:69:LEU:HB3	1:Q:137:ILE:HG22	1.78	0.66
1:O:528:ILE:N	1:O:528:ILE:HD12	2.10	0.66
1:N:480:GLU:OE2	1:N:482:HIS:CD2	2.45	0.66
1:M:83:ALA:HB1	1:M:112:TRP:CG	2.30	0.66
1:I:541:VAL:HG23	1:I:601:PRO:HG3	1.78	0.66
1:J:67:HIS:CE1	1:J:89:LYS:HD3	2.31	0.66
1:M:84:ARG:HD3	1:M:112:TRP:CH2	2.31	0.66
1:N:39:ASP:OD2	1:N:298:ARG:HD3	1.95	0.66
1:P:146:LEU:HB3	1:P:271:TRP:CD1	2.31	0.66
1:J:601:PRO:HD2	4:J:812:HOH:O	1.95	0.66
1:A:218:LEU:H	1:A:303:GLN:NE2	1.94	0.66
1:E:490:PRO:HB3	1:E:569:MET:HE3	1.77	0.66
1:K:349:LEU:HD11	1:K:353:LEU:HD12	1.78	0.66
1:F:171:PRO:HB3	1:F:273:ILE:HD12	1.76	0.66
1:N:242:HIS:O	1:N:245:LYS:HG2	1.94	0.65
1:G:559:SER:OG	1:G:632:LYS:HB2	1.95	0.65
1:O:218:LEU:HD13	1:O:268:LEU:HD13	1.78	0.65
1:A:269:MET:HG2	1:A:306:TYR:CE1	2.31	0.65
1:A:141:VAL:O	1:A:141:VAL:CG1	2.44	0.65
1:N:583:PHE:O	1:N:586:ILE:HG12	1.95	0.65
1:Q:85:GLU:HG3	1:Q:85:GLU:O	1.96	0.65
1:G:173:THR:HB	1:G:274:ASP:HB3	1.78	0.65
1:K:297:TRP:CD2	1:K:495:ASP:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:LEU:O	1:N:400:ALA:HB1	1.95	0.65
1:O:126:VAL:O	1:O:161:ARG:NH2	2.27	0.65
1:J:73:THR:HG22	1:J:94:GLU:HB2	1.77	0.65
1:C:314:VAL:HG21	1:C:320:PHE:CE2	2.31	0.65
1:D:67:HIS:CE1	1:D:91:THR:CG2	2.79	0.65
1:O:382:HIS:ND1	1:O:402:ARG:HD3	2.12	0.65
1:Q:84:ARG:O	1:Q:85:GLU:HB3	1.95	0.65
1:O:7:ASN:HD21	1:O:640:GLN:HE22	1.42	0.65
1:O:42:ARG:HH11	1:O:140:GLU:HG2	1.59	0.65
1:C:489:ILE:HD13	1:C:541:VAL:HG21	1.78	0.65
1:R:597:SER:HA	1:R:599:GLY:H	1.62	0.65
1:Q:421:HIS:O	1:Q:424:LYS:HD3	1.97	0.65
1:O:433:LYS:O	1:O:436:SER:HB2	1.97	0.65
1:L:168:ARG:NH2	1:L:276:ASP:O	2.28	0.65
1:D:42:ARG:HH11	1:D:140:GLU:CG	2.07	0.65
1:D:193:PRO:HA	1:D:362:ASN:ND2	2.11	0.65
1:C:262:GLY:O	1:C:314:VAL:HG12	1.96	0.65
1:A:480:GLU:OE2	1:A:482:HIS:CD2	2.49	0.65
1:K:250:GLU:HB2	1:K:326:HIS:NE2	2.12	0.65
1:J:273:ILE:HG13	1:J:275:MET:HE3	1.79	0.65
1:H:623:SER:O	1:H:624:LEU:HD23	1.97	0.65
1:K:283:ILE:HG23	1:K:298:ARG:HH21	1.62	0.65
1:G:42:ARG:HH21	1:G:43:ASN:HD21	1.44	0.65
1:D:616:THR:HG23	4:D:822:HOH:O	1.95	0.65
1:E:145:GLU:HG2	1:E:145:GLU:O	1.95	0.65
1:J:159:LEU:HA	1:J:163:ALA:HB3	1.79	0.65
1:K:217:GLN:HB2	1:K:536:GLU:HB3	1.78	0.65
1:C:314:VAL:CG2	1:C:320:PHE:HD2	2.10	0.64
1:D:169:VAL:HG22	1:D:171:PRO:O	1.97	0.64
1:Q:143:ASP:O	1:Q:145:GLU:N	2.30	0.64
1:R:168:ARG:NH1	1:R:241:GLU:OE2	2.29	0.64
1:F:368:GLN:NE2	1:F:371:LYS:HE3	2.12	0.64
1:M:359:TYR:CE2	1:M:605:LYS:HB2	2.32	0.64
1:B:392:LEU:C	1:B:392:LEU:HD23	2.17	0.64
1:Q:323:VAL:HG11	1:Q:340:LYS:HE2	1.78	0.64
1:H:378:SER:HB3	1:H:383:VAL:HG11	1.79	0.64
1:H:502:ASP:OD2	1:H:616:THR:HG21	1.98	0.64
1:D:629:LEU:HD21	1:E:438:THR:HG21	1.79	0.64
1:N:87:ALA:O	1:N:115:LYS:HE3	1.97	0.64
1:P:478:ARG:NH2	1:P:478:ARG:HG2	2.11	0.64
1:P:352:MET:HG2	1:P:412:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:ARG:O	1:I:277:ARG:HG2	1.96	0.64
1:D:111:PRO:O	1:D:112:TRP:HB2	1.97	0.64
1:Q:168:ARG:NH1	1:Q:168:ARG:HG2	2.02	0.64
1:N:39:ASP:OD2	1:N:298:ARG:HD2	1.98	0.64
1:L:317:ASN:HD22	1:L:317:ASN:H	1.44	0.64
1:N:55:ALA:H	1:N:58:LYS:HZ2	1.45	0.64
1:F:565:ASN:ND2	1:F:644:SER:HB2	2.12	0.64
1:A:63:ASP:O	1:A:63:ASP:OD1	2.16	0.64
1:R:280:THR:HG23	1:R:281:THR:H	1.63	0.64
1:N:550:ARG:H	1:N:560:GLN:HE22	1.45	0.64
1:N:50:LEU:O	1:N:54:ILE:CG2	2.46	0.64
1:P:4:GLU:O	1:R:420:ILE:HD11	1.98	0.64
1:K:218:LEU:HB2	1:K:303:GLN:HE21	1.62	0.64
1:H:61:ASN:ND2	1:H:65:LYS:O	2.28	0.64
1:G:45:LYS:O	1:G:275:MET:HG2	1.98	0.64
1:O:3:LEU:O	1:O:15:TRP:HA	1.98	0.64
1:N:462:PHE:O	1:N:466:VAL:HG23	1.98	0.64
1:C:42:ARG:HH21	1:C:43:ASN:HD21	1.46	0.64
1:R:176:VAL:HG13	1:R:236:PHE:HB2	1.80	0.64
1:J:218:LEU:H	1:J:303:GLN:NE2	1.96	0.64
1:G:474:GLY:HA3	1:G:476:GLU:OE2	1.98	0.64
1:G:218:LEU:H	1:G:303:GLN:NE2	1.96	0.64
1:B:4:GLU:OE2	1:B:13:ARG:HD3	1.98	0.64
1:K:122:ARG:HD3	1:K:124:THR:OG1	1.98	0.63
1:P:375:ASP:O	1:P:399:THR:HG21	1.97	0.63
1:A:218:LEU:HD12	1:A:303:GLN:HB2	1.80	0.63
1:P:38:LEU:HD13	1:P:498:ASN:HD22	1.63	0.63
1:K:516:GLU:HG3	1:K:520:LYS:HE3	1.79	0.63
1:C:269:MET:HG2	1:C:306:TYR:CE1	2.33	0.63
1:I:497:GLN:HE21	1:I:497:GLN:H	0.77	0.63
1:M:83:ALA:HB1	1:M:112:TRP:CB	2.28	0.63
1:I:218:LEU:HD13	1:I:268:LEU:HD13	1.80	0.63
1:P:141:VAL:O	1:P:141:VAL:HG12	1.96	0.63
1:L:450:TYR:H	1:L:459:HIS:HD2	1.45	0.63
1:L:168:ARG:HH11	1:L:168:ARG:CG	2.11	0.63
1:K:68:VAL:CG2	1:K:136:ILE:HB	2.26	0.63
1:K:46:PHE:CE2	1:K:140:GLU:HB2	2.33	0.63
1:A:480:GLU:OE2	1:A:482:HIS:HD2	1.80	0.63
1:M:43:ASN:N	1:M:43:ASN:HD22	1.96	0.63
1:H:84:ARG:O	1:H:85:GLU:HB2	1.99	0.63
1:E:103:ALA:O	1:E:107:THR:HB	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:218:LEU:H	1:O:303:GLN:HE21	1.43	0.63
1:K:624:LEU:H	1:K:624:LEU:HD12	1.64	0.63
1:I:543:GLY:HA3	1:I:568:ASN:ND2	2.14	0.63
1:R:497:GLN:HE21	1:R:497:GLN:H	1.44	0.63
1:A:109:ASN:N	1:A:109:ASN:HD22	1.96	0.63
1:Q:169:VAL:HG23	1:Q:172:SER:HA	1.79	0.63
1:B:41:ASP:O	1:B:44:ASP:N	2.30	0.63
1:L:577:MET:HE2	1:L:626:LEU:HD11	1.80	0.63
1:Q:528:ILE:HD13	1:Q:639:PHE:O	1.99	0.63
1:H:156:LYS:O	1:H:160:GLU:HG2	1.98	0.63
1:M:434:VAL:CG1	1:M:469:LEU:HD13	2.28	0.63
1:K:169:VAL:HG22	1:K:171:PRO:O	1.99	0.63
1:E:176:VAL:HG13	1:E:236:PHE:HB2	1.81	0.63
1:Q:73:THR:OG1	1:Q:76:GLY:HA2	1.98	0.63
1:C:103:ALA:O	1:C:107:THR:HB	1.99	0.63
1:I:193:PRO:HA	1:I:362:ASN:HD21	1.63	0.62
1:I:171:PRO:HB3	1:I:275:MET:CE	2.29	0.62
1:K:141:VAL:CG1	1:K:141:VAL:O	2.47	0.62
1:A:577:MET:HE1	1:A:639:PHE:CE1	2.33	0.62
1:H:42:ARG:HH21	1:H:43:ASN:HD21	1.47	0.62
1:I:534:LEU:HD11	1:I:576:PRO:HB3	1.80	0.62
1:C:353:LEU:HD22	1:C:357:THR:HG21	1.81	0.62
1:E:135:ASP:OD1	1:E:164:LYS:HD2	2.00	0.62
1:I:63:ASP:OD2	1:I:65:LYS:HB2	2.00	0.62
1:G:161:ARG:HB2	1:G:162:LEU:HD22	1.82	0.62
1:K:510:ASP:OD2	1:K:512:SER:HB3	1.99	0.62
1:I:157:GLU:HA	1:I:160:GLU:HG2	1.81	0.62
1:O:112:TRP:CZ3	1:O:509:PHE:HE1	2.18	0.62
1:I:420:ILE:CD1	1:I:428:VAL:HG22	2.29	0.62
1:R:467:GLU:HG3	1:R:556:ARG:HD2	1.81	0.62
1:I:178:ILE:HA	1:I:268:LEU:O	1.98	0.62
1:M:382:HIS:CD2	1:M:402:ARG:HG3	2.34	0.62
1:G:72:GLY:O	2:G:701:SAH:N	2.31	0.62
1:C:191:ASP:OD2	1:C:194:ARG:NH1	2.32	0.62
1:N:54:ILE:HD11	1:N:87:ALA:N	2.14	0.62
1:F:42:ARG:HH21	1:F:43:ASN:HD21	1.48	0.62
1:M:356:GLN:O	1:M:359:TYR:HB3	1.99	0.62
1:L:506:VAL:HG12	1:L:507:ASN:HD22	1.64	0.62
1:K:108:SER:O	1:K:113:SER:HB2	1.99	0.62
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.07	0.62
1:H:51:LYS:HG3	1:H:85:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ARG:HB3	1:C:201:GLU:OE1	2.00	0.62
1:R:356:GLN:O	1:R:606:GLY:HA2	2.00	0.62
1:E:274:ASP:HA	1:E:282:PHE:HD1	1.64	0.62
1:Q:379:LYS:HA	1:Q:399:THR:OG1	2.00	0.62
1:I:26:GLN:CG	1:I:30:ARG:HH12	1.99	0.62
1:J:39:ASP:OD2	1:J:298:ARG:CD	2.43	0.62
1:Q:97:LYS:HB2	1:Q:98:PRO:HD3	1.80	0.62
1:N:218:LEU:H	1:N:303:GLN:NE2	1.98	0.62
1:N:379:LYS:CA	1:N:399:THR:HG22	2.18	0.62
1:K:167:CYS:SG	1:K:168:ARG:N	2.73	0.62
1:P:227:ARG:HH12	1:P:229:LEU:HD21	1.64	0.62
1:I:176:VAL:HG22	1:I:235:ALA:HB3	1.82	0.62
1:D:622:LYS:H	1:D:622:LYS:HD3	1.64	0.62
1:I:292:LYS:HG2	1:I:293:ASN:HA	1.79	0.62
1:L:379:LYS:CA	1:L:399:THR:HG23	2.28	0.61
1:N:133:ARG:CG	1:N:164:LYS:HG3	2.29	0.61
1:G:108:SER:O	1:G:109:ASN:HB2	2.01	0.61
1:E:497:GLN:HE21	1:E:497:GLN:H	1.46	0.61
1:C:337:GLY:O	1:C:338:LYS:HD2	2.00	0.61
1:I:480:GLU:OE2	1:I:482:HIS:HD2	1.83	0.61
1:K:250:GLU:HB2	1:K:326:HIS:CD2	2.33	0.61
1:N:565:ASN:ND2	1:N:644:SER:OG	2.32	0.61
1:F:259:HIS:HD2	1:F:260:SER:OG	1.83	0.61
1:G:95:VAL:CG2	1:G:95:VAL:O	2.47	0.61
1:K:445:LEU:HD12	1:K:480:GLU:HB2	1.81	0.61
1:P:352:MET:HG2	1:P:412:PHE:CZ	2.35	0.61
1:D:622:LYS:HD3	1:D:622:LYS:N	2.15	0.61
1:F:243:GLU:HA	1:F:246:ILE:HD12	1.82	0.61
1:J:563:VAL:HG13	1:J:625:CYS:SG	2.40	0.61
1:L:577:MET:HE3	1:L:641:PHE:CZ	2.23	0.61
1:O:548:ILE:O	1:O:549:LEU:HD13	2.01	0.61
1:J:470:LYS:HD2	1:J:554:ASP:O	2.00	0.61
1:Q:417:PHE:CZ	1:Q:430:ILE:HB	2.36	0.61
1:B:39:ASP:OD2	1:B:298:ARG:CD	2.45	0.61
1:K:573:ASN:O	1:K:614:PRO:HD2	1.99	0.61
1:N:218:LEU:HD12	1:N:303:GLN:HB2	1.81	0.61
1:M:3:LEU:HD22	1:O:418:LYS:HA	1.83	0.61
1:K:77:LEU:HD22	1:K:511:LEU:HD11	1.83	0.61
1:P:550:ARG:H	1:P:560:GLN:HE22	1.47	0.61
1:G:218:LEU:H	1:G:303:GLN:HE21	1.48	0.61
1:C:5:LYS:NZ	1:C:14:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:444:VAL:CG1	1:N:479:VAL:HB	2.24	0.61
1:M:42:ARG:HA	1:M:283:ILE:HD11	1.82	0.61
1:K:475:ASP:OD1	1:K:475:ASP:N	2.33	0.61
1:C:216:VAL:O	1:C:302:MET:HG2	2.00	0.61
1:K:39:ASP:O	1:K:42:ARG:HB3	2.01	0.61
1:J:189:PHE:CE1	1:J:359:TYR:HB2	2.36	0.61
1:L:133:ARG:HB2	1:L:164:LYS:HG3	1.81	0.61
1:O:587:ASN:HD22	1:O:588:LEU:N	1.98	0.61
1:Q:460:LEU:HB3	1:Q:463:LEU:HD23	1.81	0.61
1:R:275:MET:HE1	1:R:283:ILE:HG13	1.82	0.61
1:Q:92:ALA:HB3	1:Q:118:VAL:HG23	1.83	0.61
1:E:241:GLU:HG3	1:E:277:ARG:HH21	1.65	0.61
1:J:67:HIS:HE1	1:J:91:THR:CG2	2.14	0.61
1:B:447:GLU:H	1:B:448:PRO:HA	1.64	0.61
1:M:196:ASN:HB2	1:M:201:GLU:OE2	2.01	0.61
1:Q:35:ASP:OD1	1:Q:299:ASP:HB3	2.01	0.61
1:F:218:LEU:N	1:F:303:GLN:NE2	2.34	0.60
1:Q:69:LEU:HD12	1:Q:91:THR:OG1	2.02	0.60
1:B:269:MET:HG2	1:B:306:TYR:CE2	2.35	0.60
1:J:182:GLU:HG3	1:J:263:THR:O	2.01	0.60
1:H:190:ASN:HD21	1:H:209:GLY:HA3	1.66	0.60
1:P:5:LYS:NZ	1:P:14:GLU:OE1	2.34	0.60
1:A:480:GLU:HG3	1:A:481:PRO:HA	1.84	0.60
1:E:511:LEU:O	1:E:514:PHE:N	2.30	0.60
1:O:275:MET:HE1	1:O:283:ILE:H	1.66	0.60
1:R:146:LEU:HB2	1:R:271:TRP:CD1	2.35	0.60
1:H:420:ILE:HD11	1:H:428:VAL:HG22	1.83	0.60
1:M:478:ARG:NH2	1:M:478:ARG:CG	2.50	0.60
1:K:241:GLU:HB2	1:K:277:ARG:HH21	1.65	0.60
1:I:273:ILE:CD1	1:I:275:MET:HE1	2.31	0.60
1:M:182:GLU:OE2	1:M:227:ARG:NH1	2.34	0.60
1:E:258:ALA:O	1:E:317:ASN:HA	2.01	0.60
1:P:365:PHE:O	1:P:371:LYS:HE3	2.01	0.60
1:A:291:ASN:H	1:A:292:LYS:NZ	1.99	0.60
1:C:460:LEU:HB3	1:C:463:LEU:HD23	1.83	0.60
1:R:562:CYS:SG	1:R:564:VAL:HG13	2.42	0.60
1:E:72:GLY:HA3	2:E:701:SAH:O4'	2.01	0.60
1:I:502:ASP:OD2	1:I:616:THR:HG21	2.01	0.60
1:M:143:ASP:HB3	1:M:149:GLU:OE1	2.01	0.60
1:F:196:ASN:O	1:F:198:GLU:N	2.33	0.60
1:A:45:LYS:O	1:A:275:MET:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ASP:HB3	1:B:65:LYS:NZ	2.16	0.60
1:L:577:MET:CE	1:L:626:LEU:HD11	2.31	0.60
1:R:203:PRO:HA	1:R:422:TYR:CG	2.37	0.60
1:A:185:LEU:O	1:A:188:MET:HB2	2.01	0.60
1:J:597:SER:CB	1:J:598:ALA:CB	2.77	0.60
1:C:168:ARG:NH2	1:C:276:ASP:O	2.34	0.60
1:N:54:ILE:C	1:N:58:LYS:NZ	2.55	0.60
1:J:91:THR:HG21	1:J:129:ILE:CG2	2.32	0.60
1:L:446:ALA:O	1:L:481:PRO:HD3	2.01	0.60
1:O:135:ASP:OD1	1:O:164:LYS:HD2	2.02	0.60
1:G:169:VAL:HG13	1:G:172:SER:HA	1.82	0.60
1:C:489:ILE:CD1	1:C:541:VAL:HG21	2.31	0.60
1:Q:583:PHE:HB3	1:Q:588:LEU:HD12	1.82	0.60
1:A:577:MET:CE	1:A:639:PHE:CE1	2.84	0.60
1:Q:95:VAL:HB	1:Q:122:ARG:HG3	1.84	0.60
1:J:141:VAL:O	1:J:141:VAL:HG13	2.00	0.60
1:Q:480:GLU:CG	1:Q:584:GLY:H	2.14	0.60
1:D:622:LYS:H	1:D:622:LYS:CD	2.15	0.60
1:C:547:GLU:OE1	1:C:550:ARG:NH1	2.35	0.60
1:M:218:LEU:H	1:M:303:GLN:NE2	2.00	0.60
1:I:470:LYS:O	1:I:473:HIS:O	2.20	0.60
1:N:36:MET:HA	1:N:300:HIS:CD2	2.36	0.60
1:J:243:GLU:H	1:J:243:GLU:CD	2.00	0.59
1:B:66:VAL:HG12	1:B:67:HIS:H	1.66	0.59
1:B:480:GLU:OE2	1:B:482:HIS:HD2	1.86	0.59
1:P:84:ARG:C	1:P:86:GLY:H	2.05	0.59
1:B:490:PRO:CB	1:B:569:MET:CE	2.60	0.59
1:K:373:GLU:HA	1:K:373:GLU:OE1	2.02	0.59
1:N:168:ARG:HG2	1:N:168:ARG:NH1	2.13	0.59
1:D:434:VAL:CG1	1:D:469:LEU:CD1	2.80	0.59
1:G:22:TYR:HE2	1:G:26:GLN:OE1	1.83	0.59
1:Q:550:ARG:H	1:Q:560:GLN:HE21	1.50	0.59
1:F:142:PHE:CD1	1:F:146:LEU:HD12	2.37	0.59
1:Q:77:LEU:HA	1:Q:80:LEU:HD12	1.83	0.59
1:Q:480:GLU:HG3	1:Q:584:GLY:N	2.18	0.59
1:P:310:GLU:OE2	1:P:338:LYS:HD2	2.02	0.59
1:M:492:LYS:HB2	1:M:572:SER:HA	1.84	0.59
1:B:54:ILE:O	1:B:58:LYS:HG2	2.03	0.59
1:R:175:ASN:HD21	1:R:237:LYS:HG2	1.66	0.59
1:G:434:VAL:CG1	1:G:469:LEU:HD13	2.32	0.59
1:D:379:LYS:CA	1:D:399:THR:CG2	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:ARG:HD3	1:M:112:TRP:HH2	1.66	0.59
1:P:190:ASN:ND2	1:P:209:GLY:HA3	2.17	0.59
1:Q:73:THR:O	2:Q:701:SAH:HA	2.02	0.59
1:L:126:VAL:HG11	1:L:129:ILE:HD13	1.85	0.59
1:C:291:ASN:HB3	1:C:295:TYR:HB2	1.83	0.59
1:F:451:MET:HG3	1:F:452:SER:N	2.18	0.59
1:D:143:ASP:OD2	1:D:148:GLY:HA3	2.02	0.59
1:R:556:ARG:CG	1:R:556:ARG:NH1	2.62	0.59
1:A:67:HIS:HE1	1:A:91:THR:HG23	1.66	0.59
1:A:497:GLN:N	1:A:497:GLN:NE2	2.46	0.59
1:Q:231:GLU:O	1:Q:232:PRO:C	2.39	0.59
1:I:269:MET:HG2	1:I:306:TYR:HE1	1.68	0.59
1:B:476:GLU:H	1:B:476:GLU:CD	2.05	0.59
1:N:142:PHE:CD1	1:N:146:LEU:CD1	2.85	0.59
1:H:52:THR:O	1:H:55:ALA:HB3	2.02	0.59
1:K:190:ASN:HD21	1:K:209:GLY:HA3	1.67	0.59
1:F:42:ARG:HH12	1:F:140:GLU:HG2	1.62	0.59
1:P:156:LYS:O	1:P:160:GLU:HG2	2.02	0.59
1:N:275:MET:HE1	1:N:283:ILE:N	2.17	0.59
1:P:138:VAL:HG23	1:P:170:VAL:HB	1.83	0.59
1:C:84:ARG:NH1	1:O:280:THR:HG23	2.18	0.59
1:N:54:ILE:HD11	1:N:87:ALA:H	1.67	0.59
1:B:41:ASP:O	1:B:42:ARG:C	2.41	0.59
1:M:84:ARG:HG2	1:M:85:GLU:OE1	2.01	0.59
1:Q:102:CYS:HA	1:Q:513:PHE:HE2	1.68	0.59
1:I:35:ASP:OD1	1:I:300:HIS:HD2	1.86	0.59
1:M:141:VAL:HG12	1:M:141:VAL:O	2.02	0.59
1:N:254:ARG:O	1:N:321:GLU:CA	2.49	0.59
1:M:379:LYS:CA	1:M:399:THR:CG2	2.80	0.59
1:P:5:LYS:CA	1:R:420:ILE:HD11	2.33	0.59
1:Q:583:PHE:CB	1:Q:588:LEU:HD12	2.33	0.59
1:O:67:HIS:HE1	1:O:91:THR:OG1	1.86	0.59
1:M:32:ARG:HG3	1:M:34:GLY:H	1.68	0.59
1:Q:375:ASP:HA	1:Q:399:THR:CG2	2.18	0.58
1:M:280:THR:HG23	1:M:281:THR:N	2.18	0.58
1:K:53:THR:HG22	1:K:168:ARG:HE	1.68	0.58
1:O:373:GLU:HG3	1:O:377:LEU:CD1	2.32	0.58
1:R:181:VAL:HG22	1:R:228:GLU:HA	1.85	0.58
1:B:245:LYS:HE3	1:E:337:GLY:HA2	1.85	0.58
1:Q:365:PHE:O	1:Q:371:LYS:HE3	2.03	0.58
1:Q:258:ALA:O	1:Q:259:HIS:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:241:GLU:CG	1:P:277:ARG:HH21	2.10	0.58
1:L:497:GLN:NE2	1:L:497:GLN:H	2.01	0.58
1:J:4:GLU:OE2	1:J:13:ARG:HD3	2.02	0.58
1:C:486:LEU:HD12	1:C:548:ILE:HB	1.85	0.58
1:P:367:ASN:OD1	1:P:369:LYS:HG2	2.02	0.58
1:R:491:GLU:HG2	1:R:493:PHE:CD2	2.38	0.58
1:A:434:VAL:HG12	1:A:469:LEU:CD1	2.34	0.58
1:M:37:ILE:HG21	1:M:503:VAL:HG11	1.85	0.58
1:M:176:VAL:HG21	1:M:236:PHE:HD2	1.68	0.58
1:M:490:PRO:HB3	1:M:569:MET:HE2	1.85	0.58
1:B:140:GLU:OE1	1:B:301:TRP:HZ2	1.86	0.58
1:K:39:ASP:OD1	1:K:298:ARG:NH1	2.36	0.58
1:M:110:SER:HB2	1:M:111:PRO:CD	2.31	0.58
1:N:490:PRO:HB3	1:N:569:MET:HE1	1.85	0.58
1:L:577:MET:CE	1:L:641:PHE:CZ	2.80	0.58
1:O:168:ARG:NH2	1:O:276:ASP:O	2.33	0.58
1:E:142:PHE:CD1	1:E:146:LEU:HD12	2.39	0.58
1:P:497:GLN:H	1:P:497:GLN:NE2	2.01	0.58
1:Q:497:GLN:NE2	1:Q:497:GLN:H	2.02	0.58
1:O:245:LYS:HD3	1:P:337:GLY:HA2	1.86	0.58
1:J:451:MET:HG3	1:J:452:SER:N	2.18	0.58
1:E:218:LEU:H	1:E:303:GLN:NE2	2.00	0.58
1:P:146:LEU:CD2	1:P:146:LEU:H	2.12	0.58
1:H:83:ALA:C	1:H:84:ARG:O	2.39	0.58
1:O:370:PHE:HE1	1:O:588:LEU:CD2	2.17	0.58
1:H:385:THR:HG22	4:H:820:HOH:O	2.04	0.58
1:F:522:ARG:O	1:F:526:ASP:HB2	2.04	0.58
1:R:180:PRO:HD2	1:R:230:SER:HB3	1.84	0.58
1:N:184:HIS:O	1:N:188:MET:HG3	2.03	0.58
1:N:58:LYS:CE	1:N:66:VAL:HG21	2.31	0.58
1:Q:222:LYS:CB	1:Q:224:HIS:HB3	2.33	0.58
1:E:383:VAL:HG21	1:E:445:LEU:HD22	1.84	0.58
1:M:169:VAL:HG11	1:M:241:GLU:HA	1.86	0.58
1:J:403:VAL:HB	1:J:428:VAL:HB	1.85	0.58
1:N:53:THR:O	1:N:58:LYS:NZ	2.37	0.58
1:Q:39:ASP:OD2	1:Q:298:ARG:HB3	2.04	0.58
1:H:141:VAL:O	1:H:141:VAL:HG13	2.04	0.58
1:G:385:THR:HG21	1:G:405:ILE:HG23	1.86	0.58
1:P:541:VAL:HG23	1:P:601:PRO:HG3	1.84	0.58
1:O:497:GLN:N	1:O:497:GLN:HE21	1.95	0.58
1:F:206:ARG:NH1	1:F:310:GLU:HG3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:MET:HB3	1:M:300:HIS:CG	2.39	0.58
1:F:168:ARG:HA	1:F:241:GLU:OE2	2.04	0.58
1:R:530:ASP:O	1:R:610:GLY:HA2	2.04	0.58
1:P:7:ASN:HD21	1:P:640:GLN:HE22	1.51	0.58
1:N:354:SER:OG	1:N:357:THR:OG1	2.21	0.58
1:E:317:ASN:N	1:E:317:ASN:ND2	2.41	0.58
1:G:66:VAL:CG1	1:G:87:ALA:HA	2.34	0.58
1:O:112:TRP:HZ3	1:O:509:PHE:HE1	1.52	0.58
1:R:80:LEU:HB3	1:R:509:PHE:CD1	2.39	0.58
1:I:478:ARG:HH21	1:I:478:ARG:CG	2.16	0.58
1:C:68:VAL:HB	1:C:90:VAL:HG22	1.85	0.58
1:F:373:GLU:OE2	1:F:585:GLY:N	2.26	0.58
1:Q:110:SER:HB2	1:Q:111:PRO:CD	2.34	0.58
1:L:480:GLU:OE2	1:L:482:HIS:HD2	1.87	0.58
1:B:94:GLU:OE2	2:B:701:SAH:O3'	2.22	0.57
1:E:140:GLU:HG3	1:E:140:GLU:O	2.04	0.57
1:N:242:HIS:HB3	1:N:245:LYS:CD	2.34	0.57
1:I:278:ASN:O	1:I:280:THR:N	2.37	0.57
1:M:37:ILE:HG21	1:M:503:VAL:HG13	1.85	0.57
1:O:80:LEU:HB3	1:O:509:PHE:CZ	2.38	0.57
1:I:157:GLU:HA	1:I:160:GLU:CG	2.34	0.57
1:Q:122:ARG:HH21	1:Q:124:THR:HG21	1.69	0.57
1:K:84:ARG:HB2	1:K:112:TRP:CE2	2.39	0.57
1:B:480:GLU:OE2	1:B:482:HIS:CD2	2.57	0.57
1:M:67:HIS:CD2	1:M:133:ARG:O	2.56	0.57
1:L:403:VAL:HB	1:L:428:VAL:HB	1.85	0.57
1:O:194:ARG:HG2	1:O:201:GLU:CB	2.34	0.57
1:A:490:PRO:CB	1:A:569:MET:CE	2.64	0.57
1:A:269:MET:CG	1:A:306:TYR:HE1	2.17	0.57
1:E:383:VAL:HB	1:E:443:ILE:HG23	1.84	0.57
1:J:618:LEU:HG	1:J:624:LEU:HD22	1.86	0.57
1:Q:150:GLY:O	1:Q:154:THR:OG1	2.22	0.57
1:P:45:LYS:HG2	1:P:282:PHE:O	2.04	0.57
1:K:179:VAL:HG21	1:K:270:TRP:CH2	2.39	0.57
1:J:144:THR:O	1:J:269:MET:CE	2.53	0.57
1:M:95:VAL:HG13	1:M:96:PHE:N	2.19	0.57
1:C:288:LYS:O	1:C:290:LYS:N	2.37	0.57
1:O:193:PRO:HA	1:O:362:ASN:HD21	1.69	0.57
1:G:81:MET:O	1:G:84:ARG:HB3	2.04	0.57
1:P:253:VAL:O	1:P:253:VAL:CG2	2.52	0.57
1:D:373:GLU:OE2	1:D:585:GLY:N	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:434:VAL:CG1	1:L:469:LEU:HD13	2.35	0.57
1:D:50:LEU:O	1:D:54:ILE:HG13	2.05	0.57
1:L:541:VAL:HG11	1:L:595:ILE:HD13	1.86	0.57
1:Q:239:ASP:OD1	1:Q:241:GLU:HB2	2.03	0.57
1:J:158:ALA:HA	1:J:162:LEU:CD2	2.30	0.57
1:J:274:ASP:OD2	1:J:277:ARG:HA	2.04	0.57
1:D:43:ASN:HB3	1:D:507:ASN:HD21	1.68	0.57
1:K:548:ILE:HG22	1:K:549:LEU:HD22	1.87	0.57
1:F:141:VAL:CG1	1:F:141:VAL:O	2.51	0.57
1:M:32:ARG:HG3	1:M:34:GLY:N	2.19	0.57
1:O:557:VAL:HG22	1:O:632:LYS:HB2	1.85	0.57
1:E:439:ASP:N	1:E:439:ASP:OD1	2.36	0.57
1:O:141:VAL:O	1:O:141:VAL:HG13	2.05	0.57
1:H:77:LEU:HD13	1:H:511:LEU:HD11	1.86	0.57
1:A:155:PHE:O	1:A:159:LEU:HG	2.04	0.57
1:A:168:ARG:NH2	1:A:276:ASP:O	2.37	0.57
1:J:497:GLN:N	1:J:497:GLN:NE2	2.51	0.57
1:L:239:ASP:OD1	1:L:277:ARG:NH2	2.36	0.57
1:I:169:VAL:HG22	1:I:171:PRO:O	2.04	0.57
1:Q:236:PHE:CZ	1:Q:324:CYS:HB3	2.40	0.57
1:O:419:TYR:O	1:O:420:ILE:C	2.42	0.57
1:A:291:ASN:H	1:A:292:LYS:HZ3	1.53	0.57
1:A:379:LYS:HA	1:A:399:THR:HG23	1.86	0.57
1:L:187:LYS:O	1:L:191:ASP:HB2	2.03	0.57
1:K:140:GLU:HG3	1:K:140:GLU:O	2.04	0.57
1:C:269:MET:HG2	1:C:306:TYR:HE1	1.69	0.57
1:O:173:THR:CG2	1:O:174:GLY:N	2.68	0.57
1:M:493:PHE:HA	1:M:539:GLY:HA3	1.86	0.57
1:M:353:LEU:HD22	1:M:357:THR:HG21	1.87	0.57
1:P:123:SER:HB3	2:P:701:SAH:HN62	1.69	0.57
1:O:7:ASN:HB2	1:O:14:GLU:CD	2.24	0.57
1:J:129:ILE:O	1:J:130:GLY:C	2.43	0.57
1:J:67:HIS:CE1	1:J:91:THR:CG2	2.87	0.57
1:L:56:GLU:OE1	1:L:168:ARG:HD2	2.04	0.57
1:R:622:LYS:N	1:R:622:LYS:HD2	2.17	0.57
1:O:420:ILE:HG13	1:O:421:HIS:N	2.19	0.57
1:F:506:VAL:HG12	1:F:507:ASN:HD22	1.70	0.57
1:P:221:MET:HG2	1:P:226:PHE:CD1	2.39	0.57
1:J:67:HIS:HD2	1:J:133:ARG:O	1.86	0.57
1:M:192:ILE:O	1:M:194:ARG:HD3	2.05	0.57
1:Q:356:GLN:NE2	1:Q:608:LYS:HE3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:485:VAL:HG21	1:O:547:GLU:HG2	1.87	0.57
1:O:56:GLU:O	1:O:60:GLU:HG2	2.05	0.57
1:M:541:VAL:CG2	1:M:601:PRO:HG3	2.35	0.57
1:O:77:LEU:HD13	1:O:511:LEU:HD11	1.86	0.57
1:G:480:GLU:OE2	1:G:482:HIS:HD2	1.88	0.57
1:D:111:PRO:O	1:D:112:TRP:CB	2.52	0.57
1:Q:447:GLU:N	1:Q:448:PRO:HA	2.20	0.57
1:L:193:PRO:HA	1:L:362:ASN:HD21	1.70	0.57
1:C:490:PRO:CB	1:C:569:MET:HE3	2.30	0.56
1:E:67:HIS:HE1	1:E:91:THR:CG2	2.11	0.56
1:K:283:ILE:HG23	1:K:298:ARG:NH2	2.20	0.56
1:K:356:GLN:O	1:K:359:TYR:HB3	2.04	0.56
1:P:549:LEU:HD12	1:P:560:GLN:NE2	2.18	0.56
1:N:140:GLU:OE1	1:N:301:TRP:HZ2	1.87	0.56
1:F:335:ASN:OD1	1:F:335:ASN:N	2.37	0.56
1:R:353:LEU:HD22	1:R:357:THR:HG21	1.87	0.56
1:B:68:VAL:HG22	1:B:136:ILE:HD12	1.86	0.56
1:L:460:LEU:HD21	1:L:579:MET:HE1	1.87	0.56
1:E:490:PRO:CB	1:E:569:MET:CE	2.79	0.56
1:R:622:LYS:H	1:R:622:LYS:CD	2.16	0.56
1:F:218:LEU:N	1:F:303:GLN:HE21	1.94	0.56
1:N:168:ARG:CG	1:N:168:ARG:HH11	2.13	0.56
1:B:314:VAL:HG21	1:B:320:PHE:CD1	2.40	0.56
1:M:300:HIS:CE1	1:M:301:TRP:CD2	2.93	0.56
1:K:145:GLU:HG3	1:K:331:LEU:HD22	1.87	0.56
1:L:317:ASN:ND2	1:L:317:ASN:H	2.03	0.56
1:R:45:LYS:O	1:R:275:MET:HG2	2.05	0.56
1:R:181:VAL:HG11	1:R:226:PHE:HB2	1.88	0.56
1:N:280:THR:OG1	1:N:281:THR:HG22	2.04	0.56
1:I:460:LEU:HB3	1:I:463:LEU:HD22	1.88	0.56
1:Q:491:GLU:OE1	1:Q:539:GLY:HA3	2.05	0.56
1:R:52:THR:HG21	1:R:276:ASP:HB2	1.87	0.56
1:F:383:VAL:HG13	1:F:403:VAL:HG22	1.86	0.56
1:Q:289:TRP:HE3	1:Q:289:TRP:O	1.88	0.56
1:Q:255:GLU:OE1	1:Q:319:THR:HG22	2.05	0.56
1:R:297:TRP:CE3	1:R:495:ASP:HB3	2.40	0.56
1:B:534:LEU:HD21	1:B:611:VAL:HG11	1.88	0.56
1:E:379:LYS:CA	1:E:399:THR:CG2	2.81	0.56
1:Q:516:GLU:O	1:Q:520:LYS:HG3	2.05	0.56
1:R:80:LEU:HD13	1:R:509:PHE:HB3	1.88	0.56
1:L:480:GLU:OE2	1:L:482:HIS:CD2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:616:THR:OG1	1:O:617:ALA:N	2.39	0.56
1:L:168:ARG:HH12	1:L:241:GLU:CD	2.08	0.56
1:O:624:LEU:HB2	1:O:643:LYS:HA	1.86	0.56
1:O:444:VAL:CG1	1:O:479:VAL:HA	2.35	0.56
1:M:37:ILE:CG2	1:M:503:VAL:HG13	2.36	0.56
1:K:218:LEU:CD1	1:K:268:LEU:HD22	2.36	0.56
1:M:3:LEU:O	1:M:15:TRP:HA	2.05	0.56
1:M:169:VAL:CG1	1:M:241:GLU:HA	2.35	0.56
1:Q:356:GLN:HE22	1:Q:608:LYS:HE3	1.71	0.56
1:J:556:ARG:HG2	1:J:556:ARG:O	2.04	0.56
1:L:114:ASP:N	1:L:114:ASP:OD1	2.35	0.56
1:K:133:ARG:HB2	1:K:164:LYS:HG3	1.87	0.56
1:I:141:VAL:O	1:I:141:VAL:CG1	2.52	0.56
1:C:288:LYS:C	1:C:290:LYS:H	2.08	0.56
1:K:354:SER:O	1:K:358:VAL:HG23	2.05	0.56
1:N:179:VAL:HG22	1:N:232:PRO:HA	1.87	0.56
1:F:145:GLU:HG2	1:F:331:LEU:HD22	1.87	0.56
1:C:490:PRO:HB3	1:C:569:MET:HE2	1.84	0.56
1:R:437:LEU:O	1:R:473:HIS:NE2	2.38	0.56
1:J:273:ILE:HG13	1:J:275:MET:CE	2.36	0.56
1:M:7:ASN:HB2	1:M:14:GLU:OE1	2.05	0.56
1:R:310:GLU:OE1	1:R:338:LYS:HG3	2.06	0.56
1:A:73:THR:HG22	1:A:94:GLU:HB2	1.87	0.56
1:K:30:ARG:NH1	1:K:526:ASP:OD1	2.39	0.56
1:K:502:ASP:CG	1:K:616:THR:HG21	2.25	0.56
1:C:522:ARG:O	1:C:526:ASP:HB2	2.05	0.56
1:N:57:LYS:NZ	1:N:166:GLY:O	2.39	0.56
1:H:273:ILE:CG1	1:H:275:MET:CE	2.81	0.56
1:O:505:THR:HA	1:O:509:PHE:O	2.05	0.56
1:A:218:LEU:H	1:A:303:GLN:HE21	1.52	0.56
1:L:191:ASP:OD2	1:L:194:ARG:NH1	2.38	0.56
1:I:643:LYS:O	1:I:644:SER:CB	2.54	0.56
1:C:517:ILE:HG13	1:C:518:SER:N	2.19	0.56
1:G:489:ILE:HD13	1:G:541:VAL:HG21	1.87	0.56
1:K:241:GLU:HB2	1:K:277:ARG:NH2	2.21	0.56
1:M:138:VAL:HG23	1:M:170:VAL:HB	1.88	0.56
1:C:42:ARG:HH11	1:C:140:GLU:HG2	1.71	0.56
1:F:443:ILE:HG12	1:F:445:LEU:HD13	1.87	0.56
1:F:291:ASN:HB3	1:F:295:TYR:HB2	1.88	0.56
1:N:378:SER:HB3	1:N:400:ALA:HB2	1.87	0.56
1:A:39:ASP:OD2	1:A:298:ARG:CD	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:69:LEU:HD12	1:R:70:ASP:N	2.20	0.56
1:E:480:GLU:OE2	1:E:482:HIS:HD2	1.89	0.55
1:F:163:ALA:HB1	1:F:167:CYS:SG	2.46	0.55
1:F:478:ARG:HH21	1:F:478:ARG:HG2	1.71	0.55
1:Q:569:MET:HE1	1:Q:575:ILE:HG12	1.88	0.55
1:Q:370:PHE:HE2	1:Q:588:LEU:HD21	1.71	0.55
1:M:198:GLU:HB2	1:M:201:GLU:OE2	2.06	0.55
1:F:35:ASP:O	1:F:36:MET:C	2.45	0.55
1:R:369:LYS:HE3	1:R:586:ILE:HG21	1.89	0.55
1:Q:222:LYS:HB2	1:Q:224:HIS:HB3	1.87	0.55
1:G:434:VAL:HG12	1:G:469:LEU:HD13	1.89	0.55
1:K:156:LYS:O	1:K:160:GLU:HG2	2.06	0.55
1:R:481:PRO:HG2	1:R:581:TRP:CE3	2.41	0.55
1:N:58:LYS:N	1:N:58:LYS:HE3	2.21	0.55
1:Q:180:PRO:CG	1:Q:230:SER:HB3	2.31	0.55
1:M:126:VAL:H	1:M:161:ARG:HH22	1.51	0.55
1:M:66:VAL:O	1:M:88:ASP:HB2	2.06	0.55
1:O:615:ILE:O	1:O:616:THR:C	2.45	0.55
1:L:502:ASP:OD2	1:L:616:THR:HG21	2.07	0.55
1:E:275:MET:HE1	1:E:283:ILE:HG13	1.88	0.55
1:N:348:GLY:O	1:N:415:ILE:HD11	2.07	0.55
1:B:344:TYR:O	1:B:346:VAL:HG13	2.07	0.55
1:E:72:GLY:CA	2:E:701:SAH:O4'	2.54	0.55
1:B:483:MET:HB3	1:B:582:GLU:HG3	1.87	0.55
1:B:38:LEU:HD21	1:B:503:VAL:HA	1.87	0.55
1:R:434:VAL:HG12	1:R:469:LEU:HD13	1.88	0.55
1:D:180:PRO:HB3	1:D:264:ILE:HD13	1.89	0.55
1:K:145:GLU:CG	1:K:331:LEU:HD22	2.37	0.55
1:J:137:ILE:HD11	1:J:163:ALA:HB2	1.89	0.55
1:C:460:LEU:HD22	1:C:463:LEU:HD21	1.88	0.55
1:I:478:ARG:HH21	1:I:478:ARG:HG2	1.70	0.55
1:F:385:THR:HB	1:F:405:ILE:HA	1.88	0.55
1:N:123:SER:OG	2:N:701:SAH:N6	2.38	0.55
1:G:36:MET:HA	1:G:300:HIS:CD2	2.41	0.55
1:F:218:LEU:H	1:F:303:GLN:HE22	1.48	0.55
1:L:136:ILE:HA	1:L:168:ARG:O	2.07	0.55
1:O:643:LYS:N	1:O:643:LYS:HD2	2.14	0.55
1:P:210:THR:HB	4:P:804:HOH:O	2.05	0.55
1:A:379:LYS:HA	1:A:399:THR:CG2	2.36	0.55
1:K:38:LEU:HD21	1:K:503:VAL:HA	1.89	0.55
1:Q:354:SER:HB2	3:Q:702:PO4:O3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:627:HIS:HB2	1:L:640:GLN:HB2	1.88	0.55
1:B:506:VAL:O	1:B:507:ASN:C	2.44	0.55
1:R:379:LYS:HA	1:R:399:THR:HG22	1.89	0.55
1:M:145:GLU:HG2	1:M:331:LEU:CD1	2.36	0.55
1:G:412:PHE:CE2	1:G:451:MET:HG2	2.40	0.55
1:R:80:LEU:HB3	1:R:509:PHE:CE1	2.41	0.55
1:B:239:ASP:OD2	1:B:242:HIS:HD2	1.89	0.55
1:J:222:LYS:HB2	1:J:225:GLU:HG2	1.89	0.55
1:J:497:GLN:N	1:J:497:GLN:HE21	1.96	0.55
1:C:522:ARG:HG2	1:C:526:ASP:OD2	2.07	0.55
1:E:359:TYR:C	1:E:359:TYR:CD1	2.81	0.55
1:H:218:LEU:H	1:H:303:GLN:HE21	1.55	0.55
1:N:367:ASN:O	1:N:371:LYS:HD3	2.07	0.55
1:Q:42:ARG:HH11	1:Q:140:GLU:HG2	1.67	0.55
1:J:383:VAL:CG2	1:J:445:LEU:HD22	2.37	0.55
1:N:315:GLU:HB2	1:N:318:GLN:CG	2.35	0.55
1:M:434:VAL:CG1	1:M:469:LEU:CD1	2.85	0.55
1:C:550:ARG:H	1:C:560:GLN:HE22	1.54	0.55
1:F:143:ASP:OD1	1:F:143:ASP:N	2.37	0.55
1:D:42:ARG:HH21	1:D:43:ASN:HD21	1.54	0.54
1:N:142:PHE:HD1	1:N:146:LEU:HD12	1.69	0.54
1:C:502:ASP:OD2	1:C:616:THR:CG2	2.55	0.54
1:R:460:LEU:HD21	1:R:579:MET:CE	2.37	0.54
1:D:157:GLU:HA	1:D:160:GLU:HG3	1.90	0.54
1:M:568:ASN:N	1:M:568:ASN:HD22	2.05	0.54
1:N:132:SER:HB2	1:R:104:ARG:CZ	2.36	0.54
1:L:297:TRP:CD2	1:L:495:ASP:HB3	2.42	0.54
1:B:550:ARG:H	1:B:560:GLN:NE2	1.99	0.54
1:B:241:GLU:HB2	1:B:277:ARG:NH2	2.21	0.54
1:M:402:ARG:NH2	1:M:429:GLU:OE1	2.28	0.54
1:C:84:ARG:NH1	1:O:280:THR:CG2	2.70	0.54
1:I:353:LEU:HD22	1:I:357:THR:HG21	1.88	0.54
1:B:554:ASP:O	1:B:555:GLY:O	2.26	0.54
1:E:420:ILE:HD11	1:E:428:VAL:HG22	1.90	0.54
1:D:565:ASN:HD21	1:D:644:SER:HB3	1.71	0.54
1:B:218:LEU:H	1:B:303:GLN:HE21	1.52	0.54
1:B:534:LEU:HD11	1:B:611:VAL:HG13	1.90	0.54
1:J:339:ASP:OD1	1:J:341:SER:HB2	2.06	0.54
1:M:486:LEU:HD22	1:M:578:TRP:O	2.07	0.54
1:R:156:LYS:HG3	1:R:157:GLU:N	2.22	0.54
1:E:39:ASP:OD2	1:E:298:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:ILE:HG21	1:J:154:THR:CG2	2.37	0.54
1:I:534:LEU:CD1	1:I:576:PRO:HB3	2.37	0.54
1:O:182:GLU:OE1	1:O:263:THR:HG22	2.07	0.54
1:M:485:VAL:HG13	1:M:487:LYS:HG3	1.88	0.54
1:O:180:PRO:HB2	1:O:264:ILE:HG12	1.89	0.54
1:P:470:LYS:O	1:P:473:HIS:O	2.26	0.54
1:P:50:LEU:O	1:P:54:ILE:HB	2.06	0.54
1:K:578:TRP:CG	1:K:591:GLY:HA3	2.43	0.54
1:N:169:VAL:CG1	1:N:240:PHE:O	2.51	0.54
1:B:43:ASN:N	1:B:43:ASN:ND2	2.55	0.54
1:K:485:VAL:HG13	1:K:487:LYS:HG3	1.90	0.54
1:P:5:LYS:HA	1:R:420:ILE:CD1	2.36	0.54
1:I:269:MET:HG2	1:I:306:TYR:CE1	2.42	0.54
1:H:420:ILE:CD1	1:H:428:VAL:HG22	2.37	0.54
1:K:556:ARG:CZ	1:K:556:ARG:H	2.20	0.54
1:C:55:ALA:HB1	1:O:292:LYS:HE3	1.90	0.54
1:R:179:VAL:HG22	1:R:232:PRO:HA	1.88	0.54
1:I:129:ILE:HG22	1:I:130:GLY:O	2.06	0.54
1:C:467:GLU:HG3	1:C:555:GLY:O	2.07	0.54
1:B:505:THR:HA	1:B:509:PHE:O	2.06	0.54
1:I:497:GLN:CD	1:I:573:ASN:ND2	2.59	0.54
1:K:84:ARG:O	1:K:85:GLU:CB	2.56	0.54
1:I:539:GLY:O	1:I:540:ILE:HD13	2.07	0.54
1:G:432:GLU:HG2	1:G:433:LYS:HG3	1.89	0.54
1:E:216:VAL:HG23	1:E:217:GLN:N	2.21	0.54
1:P:379:LYS:HA	1:P:399:THR:CG2	2.37	0.54
1:N:84:ARG:HB3	1:N:112:TRP:CZ2	2.43	0.54
1:B:194:ARG:HD2	1:B:198:GLU:O	2.08	0.54
1:B:123:SER:O	1:B:125:ASP:N	2.41	0.54
1:M:169:VAL:HG11	1:M:240:PHE:O	2.08	0.54
1:P:110:SER:HB2	1:P:112:TRP:CE3	2.43	0.54
1:P:33:PHE:HB2	1:P:36:MET:HE2	1.89	0.54
1:N:137:ILE:O	1:N:169:VAL:HA	2.08	0.54
1:L:168:ARG:NH1	1:L:168:ARG:HG2	2.15	0.54
1:D:46:PHE:CZ	1:D:140:GLU:HB2	2.42	0.54
1:D:291:ASN:O	1:D:292:LYS:HD3	2.08	0.54
1:O:417:PHE:CZ	1:O:430:ILE:HB	2.43	0.54
1:A:245:LYS:HD3	1:D:337:GLY:HA2	1.90	0.54
1:M:190:ASN:HD21	1:M:209:GLY:HA3	1.73	0.54
1:R:447:GLU:N	1:R:448:PRO:HA	2.23	0.54
1:M:533:SER:O	1:M:536:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:178:ILE:CD1	1:Q:235:ALA:HB2	2.35	0.54
1:N:490:PRO:HB3	1:N:569:MET:CE	2.38	0.54
1:Q:276:ASP:O	1:Q:277:ARG:CB	2.56	0.54
1:M:434:VAL:HG13	1:M:469:LEU:HD13	1.90	0.54
1:K:179:VAL:HG21	1:K:270:TRP:HH2	1.72	0.54
1:C:45:LYS:O	1:C:275:MET:HG2	2.08	0.54
1:I:489:ILE:O	1:I:576:PRO:HD2	2.08	0.53
1:Q:530:ASP:O	1:Q:610:GLY:HA2	2.09	0.53
1:J:592:LEU:HD21	1:J:595:ILE:HD11	1.90	0.53
1:O:73:THR:OG1	1:O:76:GLY:HA2	2.08	0.53
1:B:297:TRP:CZ2	1:B:299:ASP:HB2	2.43	0.53
1:O:4:GLU:OE2	1:O:13:ARG:NH1	2.42	0.53
1:E:138:VAL:HG23	1:E:170:VAL:HB	1.89	0.53
1:I:42:ARG:HH11	1:I:140:GLU:HG3	1.72	0.53
1:P:297:TRP:CE3	1:P:495:ASP:HB3	2.44	0.53
1:I:193:PRO:HA	1:I:362:ASN:ND2	2.23	0.53
1:O:229:LEU:HD13	1:O:314:VAL:HG12	1.89	0.53
1:G:141:VAL:O	1:G:141:VAL:HG12	2.08	0.53
1:B:627:HIS:CD2	1:B:627:HIS:N	2.76	0.53
1:D:243:GLU:N	1:D:243:GLU:OE1	2.30	0.53
1:J:88:ASP:O	1:J:115:LYS:HG2	2.08	0.53
1:Q:179:VAL:HG22	1:Q:232:PRO:HA	1.89	0.53
1:M:375:ASP:O	1:M:399:THR:HG21	2.09	0.53
1:M:132:SER:N	1:P:104:ARG:HH21	2.06	0.53
1:F:91:THR:HG22	1:F:117:THR:HG22	1.89	0.53
1:D:242:HIS:HB2	1:D:245:LYS:HG3	1.90	0.53
1:K:505:THR:HA	1:K:509:PHE:O	2.08	0.53
1:A:176:VAL:HG22	1:A:235:ALA:HB3	1.90	0.53
1:G:490:PRO:HB2	1:G:569:MET:HE1	1.84	0.53
1:N:55:ALA:CA	1:N:58:LYS:HZ2	2.22	0.53
1:E:241:GLU:CG	1:E:277:ARG:HH21	2.20	0.53
1:R:489:ILE:HD11	1:R:541:VAL:HG11	1.91	0.53
1:M:258:ALA:CB	1:M:314:VAL:HG13	2.38	0.53
1:E:274:ASP:HA	1:E:282:PHE:CD1	2.43	0.53
1:M:92:ALA:HB3	1:M:118:VAL:HG22	1.90	0.53
1:I:68:VAL:O	1:I:90:VAL:HA	2.08	0.53
1:K:36:MET:HA	1:K:300:HIS:CD2	2.43	0.53
1:L:528:ILE:HD13	1:L:639:PHE:O	2.08	0.53
1:F:277:ARG:C	1:F:279:GLY:H	2.12	0.53
1:A:214:PHE:CD2	1:A:305:VAL:HG22	2.44	0.53
1:G:6:ILE:HG13	1:I:426:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:534:LEU:O	1:K:536:GLU:N	2.42	0.53
1:Q:447:GLU:H	1:Q:448:PRO:HA	1.73	0.53
1:R:300:HIS:CE1	1:R:301:TRP:CD2	2.97	0.53
1:P:198:GLU:HB2	1:P:201:GLU:HG3	1.90	0.53
1:H:250:GLU:HB2	1:H:326:HIS:NE2	2.23	0.53
1:K:122:ARG:O	1:K:123:SER:C	2.45	0.53
1:K:123:SER:HB3	2:K:701:SAH:N6	2.13	0.53
1:I:379:LYS:HA	1:I:399:THR:CG2	2.33	0.53
1:E:434:VAL:HG13	1:E:469:LEU:HD13	1.91	0.53
1:N:450:TYR:H	1:N:459:HIS:CD2	2.22	0.53
1:R:144:THR:HG23	1:R:302:MET:O	2.09	0.53
1:B:75:THR:HG22	1:B:77:LEU:H	1.73	0.53
1:D:178:ILE:HA	1:D:268:LEU:O	2.09	0.53
1:D:78:LEU:O	1:D:81:MET:HB2	2.09	0.53
1:D:490:PRO:CB	1:D:569:MET:HE1	2.38	0.53
1:L:280:THR:HG23	1:L:281:THR:CG2	2.38	0.53
1:L:258:ALA:CB	1:L:314:VAL:HG13	2.39	0.53
1:J:264:ILE:HD12	1:J:312:LYS:HG3	1.90	0.53
1:D:45:LYS:HB3	1:D:275:MET:HE3	1.91	0.53
1:E:627:HIS:HB2	1:E:640:GLN:HB2	1.90	0.53
1:M:84:ARG:O	1:M:85:GLU:HB2	2.09	0.53
1:O:387:GLY:HA2	1:O:450:TYR:CE1	2.43	0.53
1:A:109:ASN:N	1:A:109:ASN:ND2	2.57	0.53
1:Q:259:HIS:CD2	1:Q:259:HIS:C	2.82	0.53
1:L:553:ILE:HD11	1:L:581:TRP:HZ3	1.73	0.53
1:F:216:VAL:O	1:F:302:MET:HG2	2.09	0.53
1:G:190:ASN:HD21	1:G:209:GLY:HA3	1.73	0.53
1:Q:392:LEU:CD1	1:Q:445:LEU:HB3	2.38	0.53
1:P:496:LEU:O	1:P:499:ILE:HG12	2.09	0.53
1:I:168:ARG:HG2	1:I:168:ARG:HH11	1.72	0.53
1:L:490:PRO:HB3	1:L:569:MET:HE2	1.76	0.53
1:N:87:ALA:CB	1:N:88:ASP:HB2	2.38	0.53
1:J:128:GLN:OE1	1:J:129:ILE:O	2.27	0.53
1:M:615:ILE:HG13	1:M:618:LEU:HD22	1.90	0.53
1:R:178:ILE:HG13	1:R:267:LEU:HD22	1.90	0.53
1:K:143:ASP:O	1:K:146:LEU:N	2.32	0.53
1:R:49:GLY:O	1:R:53:THR:OG1	2.27	0.53
1:Q:410:GLU:HG3	1:Q:413:ARG:NH2	2.23	0.53
1:B:84:ARG:HB3	1:B:112:TRP:CH2	2.44	0.53
1:M:409:ASN:OD1	1:M:411:ARG:HG2	2.09	0.53
1:J:378:SER:HB3	1:J:400:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ASN:O	1:E:280:THR:N	2.40	0.53
1:R:184:HIS:HA	1:R:187:LYS:HD3	1.90	0.53
1:K:126:VAL:HG12	1:K:162:LEU:HD11	1.90	0.53
1:Q:218:LEU:HD22	1:Q:221:MET:HE2	1.92	0.52
1:K:485:VAL:O	1:K:579:MET:HG3	2.09	0.52
1:R:157:GLU:O	1:R:160:GLU:HG2	2.09	0.52
1:M:516:GLU:HG2	1:M:520:LYS:HE3	1.90	0.52
1:J:410:GLU:OE2	1:K:19:GLU:HB3	2.09	0.52
1:D:445:LEU:HD12	1:D:480:GLU:HB2	1.91	0.52
1:I:570:SER:HB3	1:I:622:LYS:HA	1.92	0.52
1:D:269:MET:HG2	1:D:306:TYR:HE1	1.73	0.52
1:R:597:SER:HA	1:R:599:GLY:N	2.23	0.52
1:E:35:ASP:O	1:E:36:MET:C	2.46	0.52
1:O:280:THR:HG22	1:O:281:THR:HG22	1.90	0.52
1:B:567:ASP:O	1:B:568:ASN:HB2	2.09	0.52
1:J:561:LYS:O	1:J:562:CYS:HB3	2.09	0.52
1:K:45:LYS:NZ	1:K:294:ASN:HD22	2.07	0.52
1:F:239:ASP:OD2	1:F:242:HIS:HD2	1.92	0.52
1:N:39:ASP:OD1	1:N:39:ASP:C	2.47	0.52
1:E:595:ILE:HG22	1:E:599:GLY:HA2	1.90	0.52
1:O:291:ASN:OD1	1:O:294:ASN:HB2	2.10	0.52
1:R:502:ASP:OD2	1:R:616:THR:HG21	2.08	0.52
1:M:457:TRP:CD1	1:M:457:TRP:O	2.62	0.52
1:B:163:ALA:CB	1:B:167:CYS:SG	2.95	0.52
1:K:379:LYS:CA	1:K:399:THR:HG23	2.38	0.52
1:K:185:LEU:O	1:K:188:MET:HB2	2.10	0.52
1:R:593:LEU:O	1:R:594:SER:HB3	2.10	0.52
1:L:57:LYS:HG2	1:L:135:ASP:HB3	1.91	0.52
1:J:548:ILE:HD12	1:J:626:LEU:HD13	1.92	0.52
1:G:540:ILE:HD11	1:G:542:LYS:HE2	1.91	0.52
1:N:169:VAL:HG13	1:N:241:GLU:HG2	1.89	0.52
1:I:275:MET:HA	1:I:275:MET:CE	2.39	0.52
1:C:489:ILE:HG12	1:C:541:VAL:CG2	2.39	0.52
1:E:506:VAL:N	1:E:509:PHE:O	2.37	0.52
1:O:506:VAL:HG12	1:O:507:ASN:HD22	1.74	0.52
1:A:273:ILE:HG13	1:A:275:MET:HE1	1.91	0.52
1:E:218:LEU:H	1:E:303:GLN:HE21	1.55	0.52
1:F:147:ILE:HD11	1:F:331:LEU:HD13	1.91	0.52
1:F:478:ARG:CG	1:F:478:ARG:HH21	2.22	0.52
1:L:297:TRP:CE3	1:L:495:ASP:HB3	2.45	0.52
1:D:626:LEU:HD21	1:D:628:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:478:ARG:HH21	1:J:478:ARG:HG2	1.74	0.52
1:G:379:LYS:CA	1:G:399:THR:CG2	2.83	0.52
1:R:478:ARG:HG2	1:R:478:ARG:NH2	2.21	0.52
1:M:5:LYS:HD3	1:O:417:PHE:HE1	1.75	0.52
1:K:497:GLN:H	1:K:497:GLN:NE2	2.08	0.52
1:G:73:THR:OG1	1:G:76:GLY:HA2	2.09	0.52
1:A:541:VAL:HG11	1:A:595:ILE:HD13	1.91	0.52
1:D:630:PHE:CE1	1:D:635:GLY:HA2	2.44	0.52
1:N:141:VAL:HG12	1:N:141:VAL:O	2.09	0.52
1:J:91:THR:HG21	1:J:129:ILE:HG21	1.92	0.52
1:D:114:ASP:HB3	1:B:65:LYS:HZ1	1.73	0.52
1:P:7:ASN:HD21	1:P:640:GLN:NE2	2.08	0.52
1:J:144:THR:O	1:J:269:MET:HE1	2.10	0.52
1:I:643:LYS:O	1:I:644:SER:HB2	2.10	0.52
1:G:104:ARG:HB3	1:G:118:VAL:HB	1.91	0.52
1:J:169:VAL:HG23	1:J:171:PRO:O	2.10	0.52
1:R:433:LYS:HE3	1:R:436:SER:OG	2.10	0.52
1:R:291:ASN:CB	1:R:295:TYR:HB2	2.32	0.52
1:I:616:THR:O	1:I:619:ARG:HG2	2.10	0.52
1:J:71:ILE:HG12	1:J:93:LEU:HD12	1.91	0.52
1:R:35:ASP:OD2	1:R:300:HIS:HD2	1.93	0.52
1:J:406:ILE:HG12	1:J:431:ILE:HD11	1.91	0.52
1:K:529:VAL:HG12	1:K:530:ASP:O	2.10	0.52
1:K:177:TYR:HA	1:K:233:ILE:O	2.09	0.52
1:Q:216:VAL:C	1:Q:302:MET:HG2	2.29	0.52
1:R:292:LYS:HA	1:R:293:ASN:HD22	1.75	0.52
1:M:39:ASP:OD2	1:M:298:ARG:CD	2.57	0.52
1:B:218:LEU:HD12	1:B:303:GLN:HB3	1.92	0.52
1:D:547:GLU:OE2	1:D:550:ARG:NH1	2.37	0.52
1:R:280:THR:HG23	1:R:281:THR:N	2.24	0.52
1:C:73:THR:OG1	1:C:76:GLY:HA2	2.10	0.52
1:C:432:GLU:HG2	1:C:433:LYS:HG3	1.92	0.52
1:J:483:MET:HG2	1:J:550:ARG:HH21	1.75	0.52
1:N:154:THR:O	1:N:158:ALA:HB2	2.09	0.52
1:G:27:GLU:HG2	1:G:96:PHE:CZ	2.45	0.52
1:F:259:HIS:C	1:F:259:HIS:CD2	2.83	0.52
1:M:542:LYS:HG3	1:M:571:SER:HB2	1.91	0.52
1:B:460:LEU:HB3	1:B:463:LEU:HD22	1.91	0.52
1:D:135:ASP:OD1	1:D:164:LYS:HD2	2.09	0.52
1:P:94:GLU:O	1:P:120:SER:HA	2.10	0.52
1:M:73:THR:HB	1:M:92:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:LYS:NZ	1:I:398:LYS:HB3	2.25	0.51
1:M:269:MET:HG2	1:M:306:TYR:HE2	1.75	0.51
1:J:217:GLN:HB2	1:J:536:GLU:HB3	1.93	0.51
1:I:145:GLU:OE2	1:I:331:LEU:HB2	2.10	0.51
1:N:171:PRO:O	1:N:240:PHE:HD2	1.93	0.51
1:B:43:ASN:O	1:B:81:MET:CE	2.58	0.51
1:P:450:TYR:N	1:P:459:HIS:HD2	1.92	0.51
1:M:178:ILE:HG13	1:M:233:ILE:HG23	1.93	0.51
1:C:67:HIS:HE1	1:C:91:THR:CG2	2.23	0.51
1:K:139:ALA:HB3	1:K:155:PHE:CZ	2.45	0.51
1:I:138:VAL:HG23	1:I:170:VAL:HB	1.92	0.51
1:I:337:GLY:HA2	1:K:245:LYS:HD3	1.92	0.51
1:M:550:ARG:H	1:M:560:GLN:HE22	1.58	0.51
1:I:3:LEU:HB2	1:I:16:VAL:HG12	1.93	0.51
1:B:41:ASP:O	1:B:43:ASN:N	2.43	0.51
1:M:447:GLU:N	1:M:448:PRO:HA	2.26	0.51
1:M:492:LYS:O	1:M:540:ILE:N	2.38	0.51
1:O:632:LYS:HG3	1:O:633:SER:N	2.25	0.51
1:K:522:ARG:O	1:K:526:ASP:HB2	2.10	0.51
1:F:164:LYS:O	1:F:167:CYS:HB2	2.11	0.51
1:O:229:LEU:HD13	1:O:314:VAL:CG1	2.40	0.51
1:O:535:TRP:CD2	1:O:605:LYS:HG2	2.45	0.51
1:G:619:ARG:HG2	1:G:619:ARG:HH11	1.75	0.51
1:C:111:PRO:HA	1:O:47:LEU:HD13	1.92	0.51
1:N:595:ILE:CG2	1:N:599:GLY:HA2	2.40	0.51
1:Q:275:MET:HE1	1:Q:283:ILE:H	1.75	0.51
1:K:57:LYS:HA	1:K:60:GLU:HB2	1.93	0.51
1:M:449:PHE:HA	1:M:459:HIS:CD2	2.46	0.51
1:B:216:VAL:C	1:B:302:MET:HG2	2.30	0.51
1:N:217:GLN:NE2	1:N:298:ARG:O	2.31	0.51
1:L:129:ILE:O	1:L:129:ILE:HG23	2.09	0.51
1:M:190:ASN:ND2	1:M:209:GLY:HA3	2.26	0.51
1:N:517:ILE:HG13	1:N:518:SER:N	2.25	0.51
1:F:181:VAL:HG11	1:F:226:PHE:HB2	1.92	0.51
1:G:626:LEU:HG	1:G:641:PHE:CE2	2.45	0.51
1:N:63:ASP:N	1:N:64:GLY:HA2	2.25	0.51
1:K:68:VAL:O	1:K:90:VAL:HA	2.10	0.51
1:Q:232:PRO:HG3	1:Q:290:LYS:HE2	1.89	0.51
1:J:483:MET:HG2	1:J:550:ARG:NH2	2.26	0.51
1:O:450:TYR:H	1:O:459:HIS:CD2	2.18	0.51
1:M:482:HIS:HA	1:M:553:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:LYS:HG2	1:H:85:GLU:HG3	1.92	0.51
1:M:258:ALA:HB3	1:M:315:GLU:O	2.10	0.51
1:M:238:PHE:HB3	1:M:240:PHE:CE1	2.45	0.51
1:A:556:ARG:HG2	1:A:556:ARG:HH11	1.75	0.51
1:C:567:ASP:C	1:C:568:ASN:HD22	2.14	0.51
1:L:550:ARG:H	1:L:560:GLN:HE22	1.57	0.51
1:Q:302:MET:HG2	1:Q:303:GLN:H	1.75	0.51
1:M:379:LYS:HA	1:M:399:THR:HG22	1.90	0.51
1:M:83:ALA:HB2	1:M:116:ILE:HD11	1.92	0.51
1:G:95:VAL:HB	1:G:122:ARG:HG3	1.92	0.51
1:D:145:GLU:HA	1:D:269:MET:CE	2.41	0.51
1:M:356:GLN:NE2	1:M:608:LYS:HE3	2.25	0.51
1:R:638:ASN:N	1:R:638:ASN:HD22	2.09	0.51
1:O:2:PHE:CD2	1:O:520:LYS:HB3	2.46	0.51
1:D:271:TRP:CZ3	1:D:273:ILE:HG12	2.46	0.51
1:M:203:PRO:HA	1:M:422:TYR:CG	2.45	0.51
1:O:441:PRO:O	1:O:477:LEU:HD11	2.11	0.51
1:D:269:MET:HG2	1:D:306:TYR:CE1	2.45	0.51
1:O:194:ARG:HG2	1:O:201:GLU:HB3	1.93	0.51
1:A:379:LYS:O	1:A:381:LEU:HG	2.11	0.51
1:M:385:THR:CG2	4:M:802:HOH:O	2.59	0.51
1:M:616:THR:O	1:M:619:ARG:HB2	2.11	0.51
1:Q:464:TYR:O	1:Q:468:VAL:HG23	2.11	0.51
1:B:3:LEU:O	1:B:15:TRP:HA	2.11	0.51
1:H:626:LEU:HD23	1:H:627:HIS:N	2.25	0.51
1:B:94:GLU:O	1:B:120:SER:HA	2.10	0.51
1:D:478:ARG:NH2	1:D:478:ARG:HG2	2.13	0.51
1:N:326:HIS:HB2	1:N:331:LEU:HD12	1.92	0.51
1:P:379:LYS:CA	1:P:399:THR:HG23	2.37	0.51
1:E:547:GLU:OE1	1:E:550:ARG:NH1	2.44	0.51
1:R:146:LEU:HD23	1:R:147:ILE:HG23	1.93	0.51
1:F:1:MET:N	4:F:801:HOH:O	2.43	0.51
1:F:497:GLN:HE21	1:F:497:GLN:N	1.98	0.51
1:C:196:ASN:HB2	1:C:201:GLU:OE2	2.11	0.51
1:Q:243:GLU:HA	1:Q:246:ILE:HD12	1.92	0.51
1:Q:553:ILE:O	1:Q:553:ILE:CG2	2.59	0.51
1:L:412:PHE:HE2	1:L:451:MET:HG2	1.74	0.51
1:J:103:ALA:O	1:J:107:THR:HB	2.11	0.51
1:M:447:GLU:H	1:M:448:PRO:HA	1.75	0.51
1:Q:231:GLU:C	1:Q:232:PRO:O	2.49	0.51
1:C:502:ASP:OD2	1:C:616:THR:HG21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:220:GLU:HG3	1:R:536:GLU:O	2.11	0.51
1:O:173:THR:HG22	1:O:174:GLY:N	2.25	0.51
1:L:73:THR:HB	1:L:92:ALA:HB1	1.91	0.51
1:A:58:LYS:HD3	1:A:64:GLY:O	2.10	0.51
1:E:157:GLU:O	1:E:160:GLU:HG3	2.11	0.51
1:I:114:ASP:N	1:I:114:ASP:OD1	2.38	0.51
1:C:569:MET:HA	1:C:572:SER:HB2	1.93	0.50
1:K:273:ILE:HD12	1:K:275:MET:CE	2.40	0.50
1:M:142:PHE:HD2	1:M:146:LEU:HD12	1.76	0.50
1:C:233:ILE:HG12	1:C:256:ALA:HB2	1.94	0.50
1:F:446:ALA:O	1:F:481:PRO:HD3	2.12	0.50
1:P:486:LEU:HD11	1:P:577:MET:HE2	1.92	0.50
1:L:39:ASP:OD2	1:L:298:ARG:CD	2.60	0.50
1:B:173:THR:HG22	1:B:274:ASP:HB3	1.93	0.50
1:O:73:THR:HG23	1:O:74:GLY:N	2.26	0.50
1:E:107:THR:O	1:E:110:SER:OG	2.28	0.50
1:Q:550:ARG:H	1:Q:560:GLN:NE2	2.08	0.50
1:O:91:THR:HG22	1:O:117:THR:HG23	1.93	0.50
1:O:194:ARG:HG2	1:O:201:GLU:HB2	1.93	0.50
1:J:269:MET:HG2	1:J:306:TYR:HE1	1.76	0.50
1:G:522:ARG:O	1:G:526:ASP:HB2	2.10	0.50
1:A:447:GLU:N	1:A:448:PRO:HA	2.26	0.50
1:P:26:GLN:O	1:P:30:ARG:CD	2.59	0.50
1:Q:82:ALA:O	1:Q:87:ALA:HB3	2.11	0.50
1:C:42:ARG:NH2	1:C:43:ASN:HD21	2.09	0.50
1:J:300:HIS:CE1	1:J:301:TRP:CD2	2.99	0.50
1:K:65:LYS:HA	1:K:65:LYS:CE	2.41	0.50
1:M:541:VAL:HG22	1:M:601:PRO:HG3	1.92	0.50
1:K:556:ARG:H	1:K:556:ARG:NH1	2.09	0.50
1:I:627:HIS:HB2	1:I:640:GLN:HB2	1.94	0.50
1:A:101:ASP:O	1:A:105:HIS:HB2	2.11	0.50
1:C:35:ASP:O	1:C:38:LEU:N	2.44	0.50
1:N:578:TRP:CB	1:N:591:GLY:HA3	2.41	0.50
1:N:203:PRO:HA	1:N:422:TYR:CD2	2.46	0.50
1:F:289:TRP:O	1:F:290:LYS:HG2	2.11	0.50
1:L:84:ARG:HG3	1:L:112:TRP:CZ2	2.46	0.50
1:D:434:VAL:HG12	1:D:469:LEU:CD1	2.36	0.50
1:P:269:MET:HG2	1:P:306:TYR:CE1	2.40	0.50
1:R:218:LEU:HD13	1:R:268:LEU:HD13	1.93	0.50
1:K:356:GLN:HG2	1:K:357:THR:H	1.75	0.50
1:K:217:GLN:HG3	1:K:537:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:GLU:HB3	1:O:96:PHE:CZ	2.47	0.50
1:N:153:ARG:HB2	1:N:328:GLU:OE2	2.12	0.50
1:B:78:LEU:O	1:B:81:MET:HB2	2.12	0.50
1:I:566:ILE:CG2	1:I:569:MET:HE3	2.42	0.50
1:E:42:ARG:HH11	1:E:140:GLU:HG2	1.72	0.50
1:O:39:ASP:OD2	1:O:298:ARG:CD	2.54	0.50
1:K:143:ASP:O	1:K:144:THR:C	2.50	0.50
1:M:269:MET:HG3	1:M:269:MET:O	2.11	0.50
1:O:397:ALA:HA	1:O:403:VAL:HG21	1.93	0.50
1:K:103:ALA:O	1:K:107:THR:HB	2.11	0.50
1:G:457:TRP:HA	4:G:811:HOH:O	2.09	0.50
1:O:73:THR:CB	1:O:92:ALA:HB1	2.32	0.50
1:B:392:LEU:C	1:B:392:LEU:CD2	2.79	0.50
1:M:142:PHE:CD2	1:M:146:LEU:HD12	2.46	0.50
1:K:616:THR:C	1:K:618:LEU:H	2.15	0.50
1:O:353:LEU:HB3	1:O:357:THR:HB	1.94	0.50
1:R:421:HIS:O	1:R:424:LYS:HE3	2.12	0.50
1:E:161:ARG:HB3	1:E:162:LEU:HD13	1.94	0.50
1:D:528:ILE:H	1:D:528:ILE:HD12	1.76	0.50
1:Q:629:LEU:O	1:Q:637:ILE:HA	2.12	0.50
1:R:359:TYR:CZ	1:R:605:LYS:HB2	2.46	0.50
1:Q:14:GLU:HG2	1:Q:523:THR:HG21	1.93	0.50
1:I:375:ASP:O	1:I:399:THR:HG21	2.12	0.50
1:D:379:LYS:CA	1:D:399:THR:HG23	2.37	0.50
1:P:143:ASP:O	1:P:146:LEU:HA	2.12	0.50
1:O:477:LEU:O	1:O:479:VAL:HG12	2.12	0.50
1:I:168:ARG:NH1	1:I:168:ARG:HG2	2.24	0.50
1:E:222:LYS:O	1:E:225:GLU:HG2	2.12	0.50
1:L:65:LYS:HA	1:L:88:ASP:OD2	2.12	0.50
1:B:486:LEU:HD12	1:B:548:ILE:HB	1.94	0.50
1:F:489:ILE:O	1:F:576:PRO:HD2	2.12	0.50
1:J:168:ARG:NH2	1:J:276:ASP:O	2.43	0.50
1:K:487:LYS:HE3	1:K:547:GLU:HG2	1.94	0.50
1:K:84:ARG:HB2	1:K:112:TRP:NE1	2.27	0.50
1:J:625:CYS:SG	1:J:627:HIS:CD2	3.05	0.50
1:P:503:VAL:H	1:P:515:ASP:CG	2.15	0.50
1:G:273:ILE:HG13	1:G:273:ILE:O	2.10	0.50
1:N:359:TYR:C	1:N:359:TYR:CD1	2.85	0.50
1:B:339:ASP:OD1	1:B:341:SER:HB2	2.12	0.50
1:D:230:SER:OG	1:D:231:GLU:O	2.28	0.50
1:R:556:ARG:HG3	1:R:556:ARG:NH1	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ARG:HH22	1:E:276:ASP:C	2.15	0.50
1:E:56:GLU:HG3	1:E:57:LYS:N	2.25	0.50
1:Q:367:ASN:HD21	1:Q:369:LYS:HG2	1.77	0.50
1:C:244:GLU:OE2	1:C:244:GLU:CA	2.60	0.50
1:R:41:ASP:O	1:R:45:LYS:HB2	2.12	0.50
1:O:77:LEU:O	1:O:81:MET:HG3	2.11	0.50
1:J:26:GLN:O	1:J:30:ARG:HD2	2.12	0.50
1:R:612:TYR:OH	1:R:615:ILE:HD12	2.11	0.50
1:N:4:GLU:OE2	1:N:13:ARG:HD3	2.11	0.50
1:N:87:ALA:HB1	1:N:88:ASP:HB2	1.94	0.49
1:D:489:ILE:CG1	1:D:490:PRO:HD2	2.40	0.49
1:I:278:ASN:O	1:I:280:THR:CG2	2.58	0.49
1:B:67:HIS:C	1:B:67:HIS:ND1	2.64	0.49
1:R:218:LEU:O	1:R:220:GLU:N	2.44	0.49
1:A:273:ILE:HD11	1:A:283:ILE:HD12	1.93	0.49
1:C:485:VAL:CG2	1:C:547:GLU:HG3	2.42	0.49
1:J:406:ILE:HG21	1:J:434:VAL:HG22	1.94	0.49
1:B:452:SER:O	1:B:453:ALA:C	2.51	0.49
1:O:356:GLN:O	1:O:359:TYR:HB3	2.12	0.49
1:L:253:VAL:O	1:L:253:VAL:HG22	2.10	0.49
1:Q:141:VAL:HG12	1:Q:141:VAL:O	2.12	0.49
1:H:222:LYS:NZ	1:H:602:GLU:OE2	2.44	0.49
1:R:7:ASN:O	1:R:11:GLY:N	2.40	0.49
1:F:299:ASP:OD1	1:F:537:TYR:OH	2.15	0.49
1:J:69:LEU:HD12	1:J:91:THR:O	2.12	0.49
1:J:563:VAL:CG1	1:J:625:CYS:SG	3.00	0.49
1:E:403:VAL:HB	1:E:428:VAL:HB	1.94	0.49
1:A:550:ARG:H	1:A:560:GLN:NE2	2.10	0.49
1:B:141:VAL:O	1:B:141:VAL:HG12	2.12	0.49
1:A:221:MET:HE3	1:A:226:PHE:CD1	2.47	0.49
1:R:626:LEU:HD21	1:R:639:PHE:HD2	1.77	0.49
1:L:557:VAL:HG23	1:L:632:LYS:HB2	1.95	0.49
1:F:218:LEU:HD12	1:F:303:GLN:HB2	1.90	0.49
1:E:315:GLU:HB3	1:E:318:GLN:HG3	1.93	0.49
1:Q:269:MET:SD	1:Q:270:TRP:N	2.85	0.49
1:J:67:HIS:CE1	1:J:91:THR:HG22	2.43	0.49
1:M:136:ILE:HA	1:M:168:ARG:O	2.11	0.49
1:P:146:LEU:HB3	1:P:271:TRP:NE1	2.26	0.49
1:K:137:ILE:O	1:K:169:VAL:HA	2.12	0.49
1:R:51:LYS:NZ	1:R:51:LYS:CB	2.74	0.49
1:C:67:HIS:CE1	1:C:91:THR:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:ASN:HB2	1:O:201:GLU:OE2	2.12	0.49
1:H:618:LEU:HD21	1:H:642:GLY:HA2	1.95	0.49
1:L:218:LEU:H	1:L:303:GLN:HE21	1.60	0.49
1:P:354:SER:O	1:P:358:VAL:HG23	2.12	0.49
1:Q:114:ASP:N	1:Q:114:ASP:OD1	2.44	0.49
1:B:629:LEU:HG	1:B:629:LEU:O	2.12	0.49
1:B:37:ILE:O	1:B:37:ILE:HG22	2.13	0.49
1:Q:186:LEU:O	1:Q:307:TYR:OH	2.17	0.49
1:R:261:SER:OG	1:R:316:MET:N	2.43	0.49
1:F:144:THR:HG21	1:F:215:ASP:HB3	1.93	0.49
1:C:612:TYR:CE2	1:C:614:PRO:HA	2.47	0.49
1:I:256:ALA:O	1:I:319:THR:HA	2.10	0.49
1:Q:153:ARG:NH1	1:Q:248:PHE:CZ	2.80	0.49
1:J:42:ARG:HH11	1:J:140:GLU:HG2	1.76	0.49
1:O:194:ARG:HD2	1:O:198:GLU:O	2.13	0.49
1:R:297:TRP:CD2	1:R:495:ASP:HB3	2.48	0.49
1:E:39:ASP:OD2	1:E:298:ARG:CD	2.60	0.49
1:R:143:ASP:OD2	1:R:148:GLY:HA3	2.13	0.49
1:H:138:VAL:HG23	1:H:170:VAL:HB	1.94	0.49
1:H:379:LYS:HA	1:H:399:THR:HG23	1.94	0.49
1:K:326:HIS:HB3	1:K:331:LEU:HD12	1.93	0.49
1:M:434:VAL:HG12	1:M:469:LEU:CD1	2.42	0.49
1:L:218:LEU:H	1:L:303:GLN:NE2	2.09	0.49
1:F:626:LEU:HD23	1:F:626:LEU:C	2.32	0.49
1:G:239:ASP:OD2	1:G:277:ARG:NH2	2.45	0.49
1:O:190:ASN:ND2	1:O:209:GLY:HA3	2.26	0.49
1:G:405:ILE:HB	1:G:430:ILE:HG12	1.93	0.49
1:A:375:ASP:O	1:A:399:THR:HG21	2.13	0.49
1:I:634:THR:OG1	1:I:636:ASP:HB2	2.12	0.49
1:F:67:HIS:ND1	1:F:89:LYS:HB3	2.27	0.49
1:P:451:MET:HG3	1:P:452:SER:N	2.28	0.49
1:L:241:GLU:HB2	1:L:277:ARG:NH2	2.27	0.49
1:O:624:LEU:HB2	1:O:642:GLY:O	2.11	0.49
1:H:42:ARG:NH2	1:H:43:ASN:HD21	2.09	0.49
1:C:480:GLU:HA	1:C:481:PRO:C	2.33	0.49
1:R:567:ASP:HA	1:R:623:SER:CB	2.37	0.49
1:I:35:ASP:OD1	1:I:300:HIS:CD2	2.65	0.49
1:P:349:LEU:HD11	1:P:353:LEU:HD12	1.94	0.49
1:D:406:ILE:HG12	1:D:431:ILE:HD11	1.95	0.49
1:K:493:PHE:HA	1:K:539:GLY:HA2	1.94	0.49
1:P:292:LYS:HB3	1:P:293:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:553:ILE:H	1:R:553:ILE:HD12	1.77	0.49
1:G:272:ASP:HA	1:G:283:ILE:O	2.12	0.49
1:M:569:MET:HG3	1:M:624:LEU:HD13	1.83	0.49
1:H:273:ILE:HG13	1:H:275:MET:HE1	1.90	0.49
1:N:255:GLU:HA	1:N:320:PHE:O	2.13	0.49
1:I:69:LEU:HD23	1:I:137:ILE:HG12	1.95	0.49
1:R:172:SER:HB3	1:R:241:GLU:OE2	2.12	0.49
1:L:39:ASP:OD2	1:L:298:ARG:HD3	2.13	0.49
1:Q:139:ALA:O	1:Q:142:PHE:CE1	2.65	0.49
1:O:460:LEU:C	1:O:462:PHE:N	2.65	0.49
1:R:87:ALA:O	1:R:88:ASP:C	2.51	0.49
1:R:109:ASN:HD22	1:R:109:ASN:N	2.10	0.49
1:F:45:LYS:HE2	1:F:282:PHE:O	2.12	0.49
1:H:273:ILE:CG1	1:H:275:MET:HE3	2.28	0.49
1:I:497:GLN:NE2	1:I:497:GLN:N	2.38	0.49
1:Q:443:ILE:HG13	1:Q:478:ARG:O	2.13	0.49
1:M:35:ASP:O	1:M:37:ILE:N	2.45	0.49
1:R:218:LEU:HD22	1:R:221:MET:HE2	1.94	0.49
1:F:171:PRO:CB	1:F:273:ILE:HD12	2.43	0.49
1:F:353:LEU:HD22	1:F:357:THR:HG21	1.95	0.49
1:R:42:ARG:HH11	1:R:140:GLU:HG2	1.78	0.49
1:N:28:LEU:O	1:N:31:SER:HB2	2.13	0.49
1:M:569:MET:CG	1:M:624:LEU:HD12	2.22	0.49
1:C:168:ARG:NH1	1:C:241:GLU:OE2	2.46	0.49
1:H:42:ARG:HH11	1:H:140:GLU:CG	2.22	0.49
1:J:443:ILE:HG12	1:J:445:LEU:HD13	1.95	0.49
1:B:447:GLU:N	1:B:448:PRO:CA	2.76	0.49
1:Q:643:LYS:O	1:Q:644:SER:CB	2.61	0.49
1:M:214:PHE:HD2	1:M:305:VAL:HG22	1.75	0.49
1:G:470:LYS:O	1:G:473:HIS:O	2.30	0.49
1:D:355:ARG:HD3	4:D:806:HOH:O	2.11	0.49
1:C:378:SER:HB3	1:C:400:ALA:HB2	1.95	0.49
1:P:168:ARG:HH22	1:P:276:ASP:C	2.16	0.49
1:C:15:TRP:CD2	1:C:520:LYS:HG2	2.48	0.49
1:M:278:ASN:O	1:M:280:THR:N	2.44	0.48
1:K:90:VAL:HB	1:K:116:ILE:HG12	1.94	0.48
1:R:284:ASP:HB3	1:R:291:ASN:HD21	1.78	0.48
1:I:175:ASN:O	1:I:271:TRP:HA	2.13	0.48
1:F:145:GLU:CG	1:F:331:LEU:HD22	2.42	0.48
1:O:535:TRP:CD1	1:O:605:LYS:HA	2.48	0.48
1:Q:275:MET:HE1	1:Q:283:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:467:GLU:HA	1:O:467:GLU:OE1	2.13	0.48
1:R:169:VAL:HG23	1:R:171:PRO:O	2.13	0.48
1:G:353:LEU:HD22	1:G:357:THR:HG21	1.94	0.48
1:K:299:ASP:O	1:K:301:TRP:N	2.46	0.48
1:J:490:PRO:HB2	1:J:569:MET:HE2	1.90	0.48
1:I:273:ILE:CG1	1:I:275:MET:HE1	2.43	0.48
1:D:80:LEU:HD13	1:D:509:PHE:CD1	2.48	0.48
1:A:218:LEU:HD12	1:A:303:GLN:CB	2.42	0.48
1:R:175:ASN:ND2	1:R:237:LYS:HG2	2.28	0.48
1:L:193:PRO:HA	1:L:362:ASN:ND2	2.28	0.48
1:K:316:MET:HG2	1:K:317:ASN:N	2.27	0.48
1:C:218:LEU:HD13	1:C:268:LEU:HD13	1.95	0.48
1:E:41:ASP:O	1:E:42:ARG:C	2.51	0.48
1:B:66:VAL:CG1	1:B:67:HIS:N	2.76	0.48
1:P:141:VAL:O	1:P:141:VAL:CG1	2.61	0.48
1:N:188:MET:O	1:N:362:ASN:OD1	2.31	0.48
1:C:218:LEU:H	1:C:303:GLN:HE21	1.61	0.48
1:P:500:ALA:HB1	1:P:522:ARG:HH22	1.78	0.48
1:K:444:VAL:HG13	1:K:479:VAL:HB	1.95	0.48
1:R:539:GLY:O	1:R:601:PRO:HD2	2.13	0.48
1:P:106:ILE:HD11	1:P:513:PHE:HB3	1.96	0.48
1:N:56:GLU:OE1	1:N:168:ARG:HD2	2.14	0.48
1:Q:269:MET:HG2	1:Q:306:TYR:HE1	1.79	0.48
1:M:111:PRO:C	1:M:113:SER:H	2.17	0.48
1:J:242:HIS:O	1:J:245:LYS:HB2	2.12	0.48
1:B:218:LEU:HD12	1:B:303:GLN:CB	2.43	0.48
1:R:218:LEU:C	1:R:220:GLU:H	2.16	0.48
1:M:89:LYS:HZ2	1:M:89:LYS:HB3	1.78	0.48
1:I:291:ASN:ND2	1:I:295:TYR:HA	2.29	0.48
1:C:57:LYS:HE2	1:C:135:ASP:HB3	1.95	0.48
1:C:62:THR:N	1:C:63:ASP:HB3	2.29	0.48
1:O:599:GLY:O	1:O:601:PRO:HD3	2.13	0.48
1:I:45:LYS:NZ	1:I:282:PHE:O	2.45	0.48
1:E:168:ARG:HA	1:E:241:GLU:OE2	2.13	0.48
1:O:569:MET:HA	1:O:572:SER:HB2	1.95	0.48
1:Q:570:SER:CB	1:Q:622:LYS:HD3	2.40	0.48
1:P:280:THR:HG23	1:P:281:THR:HG23	1.94	0.48
1:E:36:MET:SD	2:E:701:SAH:HG1	2.54	0.48
1:M:550:ARG:O	1:M:560:GLN:OE1	2.31	0.48
1:O:467:GLU:OE2	1:O:556:ARG:HA	2.13	0.48
1:O:297:TRP:CD2	1:O:495:ASP:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:631:ASP:O	1:P:635:GLY:N	2.41	0.48
1:C:280:THR:HG23	1:C:281:THR:HG23	1.95	0.48
1:K:273:ILE:HD12	1:K:275:MET:HE3	1.95	0.48
1:H:51:LYS:HG3	1:H:85:GLU:CG	2.43	0.48
1:Q:51:LYS:HA	1:Q:85:GLU:CD	2.33	0.48
1:O:548:ILE:O	1:O:562:CYS:SG	2.67	0.48
1:L:420:ILE:HD11	1:L:428:VAL:HG22	1.94	0.48
1:R:36:MET:HA	1:R:300:HIS:CD2	2.48	0.48
1:I:136:ILE:HA	1:I:168:ARG:O	2.13	0.48
1:L:253:VAL:O	1:L:253:VAL:CG2	2.61	0.48
1:I:543:GLY:HA3	1:I:568:ASN:HD22	1.77	0.48
1:N:84:ARG:HD2	1:N:85:GLU:HG2	1.95	0.48
1:B:178:ILE:HA	1:B:268:LEU:O	2.14	0.48
1:E:275:MET:HE1	1:E:283:ILE:H	1.78	0.48
1:J:169:VAL:CG2	1:J:171:PRO:O	2.62	0.48
1:O:535:TRP:CE3	1:O:535:TRP:O	2.67	0.48
1:D:528:ILE:N	1:D:528:ILE:HD12	2.28	0.48
1:J:308:LEU:HD13	1:J:333:PHE:O	2.13	0.48
1:I:587:ASN:C	1:I:587:ASN:ND2	2.67	0.48
1:E:226:PHE:CD1	1:E:226:PHE:N	2.81	0.48
1:C:484:GLY:HA3	1:C:581:TRP:CZ3	2.49	0.48
1:L:290:LYS:HG2	1:L:290:LYS:O	2.13	0.48
1:D:489:ILE:O	1:D:576:PRO:HD2	2.13	0.48
1:N:387:GLY:HA2	1:N:450:TYR:CE2	2.48	0.48
1:N:84:ARG:O	1:N:85:GLU:HB2	2.14	0.48
1:J:193:PRO:HA	1:J:362:ASN:ND2	2.26	0.48
1:E:75:THR:O	1:E:103:ALA:HA	2.13	0.48
1:N:42:ARG:NH1	1:N:140:GLU:HG2	2.28	0.48
1:R:338:LYS:HD3	1:R:338:LYS:HA	1.52	0.48
1:O:553:ILE:HG13	1:O:554:ASP:H	1.79	0.48
1:P:228:GLU:OE2	1:P:290:LYS:NZ	2.47	0.48
1:P:455:ASN:HB2	1:P:458:ASN:HB2	1.96	0.48
1:A:467:GLU:CD	1:A:557:VAL:HG12	2.34	0.48
1:I:273:ILE:HG13	1:I:283:ILE:HB	1.96	0.48
1:B:218:LEU:HD13	1:B:268:LEU:HD13	1.96	0.48
1:M:300:HIS:CE1	1:M:301:TRP:CE2	3.02	0.48
1:K:145:GLU:HG3	1:K:331:LEU:CD2	2.44	0.48
1:K:220:GLU:HG3	1:K:536:GLU:O	2.13	0.48
1:Q:143:ASP:C	1:Q:145:GLU:H	2.17	0.48
1:K:218:LEU:HD13	1:K:268:LEU:HD22	1.95	0.48
1:R:548:ILE:HG22	1:R:549:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:356:GLN:O	1:Q:359:TYR:HB3	2.13	0.48
1:B:460:LEU:HD21	1:B:579:MET:CE	2.44	0.48
1:E:388:GLU:OE1	1:E:452:SER:HB2	2.13	0.48
1:M:159:LEU:HD13	1:M:243:GLU:N	2.29	0.48
1:H:38:LEU:HD21	1:H:503:VAL:HA	1.96	0.48
1:N:405:ILE:HB	1:N:430:ILE:HG12	1.95	0.48
1:D:443:ILE:HG13	1:D:478:ARG:HB3	1.95	0.48
1:O:382:HIS:HD2	1:O:441:PRO:HA	1.73	0.48
1:K:297:TRP:CE3	1:K:495:ASP:HB3	2.48	0.48
1:G:56:GLU:C	1:G:58:LYS:H	2.16	0.48
1:C:293:ASN:N	1:C:293:ASN:OD1	2.46	0.48
1:O:522:ARG:O	1:O:526:ASP:HB2	2.14	0.48
1:F:497:GLN:NE2	1:F:497:GLN:N	2.59	0.47
1:N:67:HIS:HB3	1:N:135:ASP:H	1.79	0.47
1:I:615:ILE:O	1:I:616:THR:C	2.52	0.47
1:P:72:GLY:O	2:P:701:SAH:N	2.42	0.47
1:P:531:GLU:HA	1:P:609:GLN:O	2.14	0.47
1:H:20:GLU:HG3	1:H:20:GLU:H	1.52	0.47
1:O:375:ASP:HB3	1:O:399:THR:OG1	2.14	0.47
1:D:578:TRP:CG	1:D:591:GLY:HA3	2.49	0.47
1:A:612:TYR:CE2	1:A:614:PRO:HA	2.49	0.47
1:K:291:ASN:HB3	1:K:295:TYR:HB2	1.96	0.47
1:Q:489:ILE:HG22	1:Q:578:TRP:HZ3	1.79	0.47
1:N:339:ASP:HA	1:Q:244:GLU:HG3	1.96	0.47
1:C:323:VAL:HG12	1:C:325:ASN:HD21	1.79	0.47
1:M:271:TRP:O	1:M:285:MET:HB2	2.14	0.47
1:M:497:GLN:HE21	1:M:497:GLN:N	1.99	0.47
1:Q:236:PHE:CE2	1:Q:326:HIS:HD2	2.32	0.47
1:D:67:HIS:HE1	1:D:91:THR:HG22	1.77	0.47
1:N:84:ARG:CB	1:N:112:TRP:CZ2	2.97	0.47
1:D:239:ASP:OD2	1:D:242:HIS:HD2	1.96	0.47
1:D:22:TYR:CE2	1:D:525:THR:HG22	2.50	0.47
1:O:85:GLU:HA	1:O:85:GLU:OE1	2.14	0.47
1:D:435:THR:HA	1:D:472:MET:SD	2.54	0.47
1:D:202:GLU:HA	4:D:852:HOH:O	2.14	0.47
1:L:385:THR:HG22	4:L:825:HOH:O	2.13	0.47
1:N:180:PRO:HB2	1:N:264:ILE:HG12	1.96	0.47
1:G:489:ILE:HG13	1:G:490:PRO:HD2	1.95	0.47
1:F:140:GLU:HG3	1:F:140:GLU:O	2.14	0.47
1:O:218:LEU:H	1:O:303:GLN:HE22	1.57	0.47
1:R:291:ASN:O	1:R:292:LYS:HD2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:PRO:HG2	1:M:112:TRP:CE3	2.48	0.47
1:C:480:GLU:OE2	1:C:482:HIS:CD2	2.55	0.47
1:H:51:LYS:NZ	1:H:51:LYS:CB	2.78	0.47
1:K:353:LEU:HD22	1:K:357:THR:HG21	1.95	0.47
1:K:532:GLN:HB2	1:K:532:GLN:HE21	1.45	0.47
1:L:317:ASN:ND2	1:L:317:ASN:N	2.63	0.47
1:H:218:LEU:HD13	1:H:268:LEU:HD13	1.96	0.47
1:J:270:TRP:CE2	1:J:286:GLY:HA2	2.49	0.47
1:J:356:GLN:O	1:J:606:GLY:HA2	2.14	0.47
1:M:507:ASN:N	1:M:507:ASN:HD22	2.11	0.47
1:Q:357:THR:O	1:Q:361:VAL:HG23	2.15	0.47
1:B:491:GLU:HG3	1:B:492:LYS:N	2.29	0.47
1:M:250:GLU:HB2	1:M:326:HIS:CD2	2.49	0.47
1:A:76:GLY:O	1:A:77:LEU:C	2.53	0.47
1:C:28:LEU:HD23	1:C:521:ALA:HB2	1.95	0.47
1:F:42:ARG:HH21	1:F:43:ASN:ND2	2.11	0.47
1:J:450:TYR:H	1:J:459:HIS:CD2	2.20	0.47
1:O:168:ARG:HG2	1:O:241:GLU:OE2	2.14	0.47
1:K:412:PHE:CE2	1:K:451:MET:HG2	2.44	0.47
1:G:478:ARG:NH2	1:G:480:GLU:OE1	2.47	0.47
1:E:157:GLU:HA	1:E:160:GLU:CG	2.45	0.47
1:A:243:GLU:HG2	1:A:244:GLU:OE1	2.14	0.47
1:K:193:PRO:HA	1:K:362:ASN:ND2	2.28	0.47
1:R:643:LYS:O	1:R:644:SER:HB3	2.15	0.47
1:E:284:ASP:HB3	1:E:294:ASN:HB2	1.96	0.47
1:B:535:TRP:CE3	1:B:605:LYS:HE3	2.49	0.47
1:O:146:LEU:HB2	1:O:271:TRP:CD1	2.49	0.47
1:K:489:ILE:HD12	1:K:545:ALA:HB2	1.95	0.47
1:K:196:ASN:HB2	1:K:201:GLU:OE2	2.15	0.47
1:J:490:PRO:HB2	1:J:572:SER:OG	2.14	0.47
1:R:218:LEU:N	1:R:303:GLN:HE21	2.11	0.47
1:B:507:ASN:HD22	1:B:507:ASN:N	2.13	0.47
1:H:277:ARG:O	1:H:277:ARG:HG2	2.13	0.47
1:F:250:GLU:OE2	1:F:252:PHE:CE2	2.68	0.47
1:R:437:LEU:HD13	1:R:441:PRO:HD3	1.95	0.47
1:E:567:ASP:OD1	1:E:623:SER:OG	2.29	0.47
1:I:420:ILE:HD11	1:I:428:VAL:HG22	1.95	0.47
1:R:548:ILE:HD12	1:R:564:VAL:HG21	1.96	0.47
1:O:556:ARG:O	1:O:558:SER:OG	2.30	0.47
1:B:470:LYS:NZ	1:B:553:ILE:O	2.47	0.47
1:G:112:TRP:HD1	1:G:115:LYS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:243:GLU:CD	1:R:243:GLU:H	2.16	0.47
1:A:623:SER:O	1:A:624:LEU:HD23	2.15	0.47
1:N:625:CYS:HB2	1:N:643:LYS:O	2.13	0.47
1:L:61:ASN:O	1:L:63:ASP:O	2.33	0.47
1:J:143:ASP:HB3	1:J:149:GLU:HG3	1.95	0.47
1:I:297:TRP:CD2	1:I:495:ASP:HB3	2.50	0.47
1:H:497:GLN:N	1:H:497:GLN:NE2	2.43	0.47
1:P:387:GLY:HA2	1:P:450:TYR:CE1	2.50	0.47
1:D:379:LYS:HA	1:D:399:THR:HG22	1.92	0.47
1:H:450:TYR:N	1:H:459:HIS:HD2	2.02	0.47
1:M:181:VAL:HG21	1:M:268:LEU:CD1	2.37	0.47
1:I:137:ILE:O	1:I:169:VAL:HA	2.15	0.47
1:R:375:ASP:OD1	1:R:375:ASP:N	2.48	0.47
1:A:480:GLU:HA	1:A:481:PRO:C	2.34	0.47
1:E:108:SER:O	1:E:110:SER:N	2.47	0.47
1:O:587:ASN:C	1:O:587:ASN:HD22	2.18	0.47
1:M:540:ILE:HD12	1:M:542:LYS:HE2	1.97	0.47
1:R:69:LEU:HD11	1:R:71:ILE:HG12	1.97	0.47
1:M:568:ASN:N	1:M:568:ASN:ND2	2.62	0.47
1:D:218:LEU:H	1:D:303:GLN:HE21	1.62	0.47
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.29	0.47
1:C:35:ASP:O	1:C:36:MET:C	2.53	0.47
1:O:539:GLY:O	1:O:601:PRO:HD2	2.14	0.47
1:E:451:MET:HG3	1:E:452:SER:N	2.28	0.47
1:E:71:ILE:HG23	1:E:93:LEU:HD12	1.96	0.47
1:F:316:MET:HA	1:F:317:ASN:HA	1.63	0.47
1:Q:438:THR:HG21	1:R:629:LEU:HD21	1.97	0.47
1:C:261:SER:OG	1:C:316:MET:N	2.47	0.47
1:A:452:SER:O	1:A:453:ALA:C	2.53	0.47
1:J:444:VAL:HG13	1:J:479:VAL:HB	1.96	0.47
1:R:13:ARG:HB2	1:R:13:ARG:NH1	2.30	0.47
1:M:179:VAL:HG22	1:M:232:PRO:HA	1.96	0.47
1:B:258:ALA:O	1:B:316:MET:HA	2.14	0.47
1:N:325:ASN:HB2	1:N:332:TRP:CE2	2.50	0.47
1:O:177:TYR:O	1:O:269:MET:HA	2.14	0.47
1:D:278:ASN:HB2	1:D:280:THR:HG22	1.95	0.47
1:B:78:LEU:HD22	2:B:701:SAH:HN2	1.80	0.47
1:Q:478:ARG:CG	1:Q:478:ARG:HH21	2.20	0.47
1:M:95:VAL:CB	1:M:122:ARG:HG3	2.44	0.47
1:R:604:ASN:OD1	1:R:606:GLY:N	2.33	0.47
1:P:367:ASN:HD21	1:P:369:LYS:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:LYS:O	1:E:275:MET:HG2	2.15	0.47
1:N:43:ASN:HD22	1:N:43:ASN:N	2.12	0.47
1:N:57:LYS:HB3	1:N:66:VAL:HG11	1.97	0.47
1:K:168:ARG:HH11	1:K:168:ARG:HG2	1.80	0.47
1:G:375:ASP:O	1:G:399:THR:HG21	2.14	0.47
1:I:177:TYR:HA	1:I:233:ILE:O	2.14	0.47
1:N:275:MET:HE2	1:N:275:MET:H	1.79	0.47
1:R:84:ARG:O	1:R:85:GLU:HB2	2.15	0.47
1:F:416:PHE:O	1:F:420:ILE:HG13	2.15	0.47
1:R:354:SER:O	1:R:358:VAL:HG23	2.14	0.47
1:R:578:TRP:HE1	1:R:580:GLU:HG3	1.80	0.47
1:A:241:GLU:HG3	1:A:277:ARG:HH21	1.79	0.47
1:I:566:ILE:HG22	1:I:569:MET:HE3	1.97	0.47
1:J:129:ILE:O	1:J:131:GLY:N	2.47	0.47
1:M:111:PRO:HG2	1:M:112:TRP:CZ3	2.50	0.47
1:D:292:LYS:HA	1:D:293:ASN:HA	1.53	0.47
1:M:615:ILE:O	1:M:615:ILE:HG13	2.14	0.47
1:Q:222:LYS:HB3	1:Q:224:HIS:HB3	1.96	0.47
1:K:181:VAL:HG21	1:K:268:LEU:HD11	1.97	0.47
1:R:35:ASP:O	1:R:36:MET:C	2.53	0.47
1:N:514:PHE:O	1:N:518:SER:CB	2.63	0.47
1:P:529:VAL:HG12	1:P:530:ASP:O	2.15	0.47
1:R:97:LYS:HB2	1:R:98:PRO:HD3	1.96	0.47
1:G:179:VAL:HG22	1:G:232:PRO:HA	1.96	0.47
1:I:298:ARG:HD2	1:I:301:TRP:HE3	1.80	0.47
1:B:416:PHE:O	1:B:420:ILE:HG13	2.15	0.47
1:F:57:LYS:HG2	1:F:135:ASP:HB3	1.97	0.47
1:Q:179:VAL:HG21	1:Q:270:TRP:CH2	2.51	0.46
1:I:146:LEU:HB2	1:I:271:TRP:CD1	2.50	0.46
1:H:137:ILE:O	1:H:169:VAL:HA	2.15	0.46
1:E:84:ARG:HG3	1:E:85:GLU:N	2.31	0.46
1:G:483:MET:SD	1:G:550:ARG:HG3	2.55	0.46
1:K:180:PRO:O	1:K:181:VAL:HG23	2.16	0.46
1:F:259:HIS:O	1:F:259:HIS:CD2	2.68	0.46
1:Q:460:LEU:HD22	1:Q:463:LEU:HD21	1.97	0.46
1:E:216:VAL:O	1:E:302:MET:HG2	2.16	0.46
1:C:73:THR:O	2:C:701:SAH:HA	2.15	0.46
1:N:595:ILE:HG22	1:N:599:GLY:HA2	1.97	0.46
1:L:412:PHE:CE2	1:L:451:MET:HG2	2.49	0.46
1:O:269:MET:HG3	1:O:304:ALA:HB3	1.97	0.46
1:R:580:GLU:HA	1:R:588:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:O	1:B:60:GLU:C	2.52	0.46
1:G:492:LYS:HB2	1:G:571:SER:O	2.14	0.46
1:F:449:PHE:C	1:F:449:PHE:CD1	2.89	0.46
1:P:285:MET:O	1:P:303:GLN:OE1	2.33	0.46
1:G:57:LYS:NZ	1:G:166:GLY:O	2.48	0.46
1:N:512:SER:O	1:N:515:ASP:HB2	2.15	0.46
1:B:516:GLU:HG2	1:B:517:ILE:N	2.30	0.46
1:P:407:ASP:O	1:P:413:ARG:HD3	2.15	0.46
1:E:258:ALA:HB2	1:E:314:VAL:HG13	1.98	0.46
1:N:56:GLU:O	1:N:60:GLU:HG3	2.14	0.46
1:B:297:TRP:CE3	1:B:298:ARG:HA	2.50	0.46
1:N:27:GLU:HB3	1:N:96:PHE:CE1	2.50	0.46
1:O:419:TYR:O	1:O:422:TYR:N	2.44	0.46
1:R:53:THR:HB	1:R:136:ILE:HD13	1.96	0.46
1:F:198:GLU:O	1:F:201:GLU:HG3	2.16	0.46
1:K:104:ARG:HA	1:K:107:THR:HG22	1.98	0.46
1:J:381:LEU:HD23	1:J:381:LEU:HA	1.73	0.46
1:E:179:VAL:HG11	1:E:228:GLU:HG2	1.97	0.46
1:B:434:VAL:HG12	1:B:469:LEU:HD13	1.97	0.46
1:E:406:ILE:HG12	1:E:431:ILE:HD11	1.97	0.46
1:C:168:ARG:CG	1:C:168:ARG:NH1	2.52	0.46
1:I:271:TRP:HZ3	1:I:283:ILE:HG22	1.79	0.46
1:G:550:ARG:H	1:G:560:GLN:HE22	1.64	0.46
1:M:94:GLU:OE2	2:M:701:SAH:H1'	2.15	0.46
1:O:84:ARG:HG3	1:O:112:TRP:CZ2	2.50	0.46
1:N:549:LEU:HD12	1:N:560:GLN:NE2	2.30	0.46
1:K:218:LEU:HD11	1:K:268:LEU:HD22	1.98	0.46
1:R:181:VAL:CG1	1:R:226:PHE:HB2	2.45	0.46
1:H:178:ILE:HA	1:H:268:LEU:O	2.15	0.46
1:I:398:LYS:HZ3	1:I:398:LYS:HB3	1.81	0.46
1:E:242:HIS:HB3	1:E:244:GLU:OE2	2.15	0.46
1:G:75:THR:O	1:G:106:ILE:HD12	2.15	0.46
1:N:160:GLU:H	1:N:160:GLU:HG2	1.55	0.46
1:N:553:ILE:HA	1:N:553:ILE:HD12	1.72	0.46
1:J:51:LYS:HG3	1:J:85:GLU:CD	2.34	0.46
1:F:360:HIS:NE2	1:F:447:GLU:OE2	2.40	0.46
1:C:70:ASP:HA	1:C:138:VAL:O	2.14	0.46
1:R:480:GLU:OE2	1:R:482:HIS:HD2	1.97	0.46
1:F:107:THR:HG21	1:F:116:ILE:HG21	1.97	0.46
1:M:381:LEU:HB3	1:M:442:ASP:HB2	1.97	0.46
1:Q:254:ARG:O	1:Q:321:GLU:CA	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLU:HB2	1:H:326:HIS:CD2	2.51	0.46
1:Q:392:LEU:HD12	1:Q:445:LEU:HB3	1.97	0.46
1:R:553:ILE:N	1:R:553:ILE:HD12	2.29	0.46
1:O:38:LEU:HD21	1:O:503:VAL:HA	1.96	0.46
1:K:28:LEU:HD11	1:K:517:ILE:HD12	1.98	0.46
1:M:175:ASN:HD21	1:M:237:LYS:NZ	2.13	0.46
1:Q:522:ARG:O	1:Q:526:ASP:HB2	2.14	0.46
1:O:498:ASN:HA	1:O:501:SER:OG	2.15	0.46
1:O:410:GLU:HG3	1:O:410:GLU:O	2.14	0.46
1:I:555:GLY:HA3	1:I:556:ARG:O	2.14	0.46
1:C:144:THR:O	1:C:271:TRP:CD1	2.68	0.46
1:M:193:PRO:HA	1:M:362:ASN:HD21	1.81	0.46
1:J:175:ASN:ND2	1:J:237:LYS:HG2	2.31	0.46
1:P:157:GLU:O	1:P:161:ARG:HB2	2.15	0.46
1:F:73:THR:O	1:F:74:GLY:C	2.54	0.46
1:F:169:VAL:HG22	1:F:241:GLU:HG2	1.97	0.46
1:P:45:LYS:HZ1	1:P:294:ASN:HD22	1.61	0.46
1:H:218:LEU:H	1:H:303:GLN:NE2	2.12	0.46
1:M:483:MET:HE3	1:M:550:ARG:HG2	1.96	0.46
1:R:140:GLU:HG3	1:R:140:GLU:O	2.16	0.46
1:A:244:GLU:CD	1:A:244:GLU:H	2.18	0.46
1:P:447:GLU:N	1:P:448:PRO:HA	2.30	0.46
1:R:258:ALA:C	1:R:260:SER:H	2.19	0.46
1:G:144:THR:HG23	1:G:302:MET:O	2.16	0.46
1:G:258:ALA:HB3	1:G:315:GLU:O	2.15	0.46
1:N:349:LEU:HD23	1:N:350:HIS:N	2.30	0.46
1:Q:420:ILE:HD11	1:R:5:LYS:HA	1.98	0.46
1:N:379:LYS:CA	1:N:399:THR:CG2	2.86	0.46
1:C:56:GLU:OE1	1:C:168:ARG:HD2	2.16	0.46
1:E:67:HIS:CE1	1:E:91:THR:CG2	2.88	0.46
1:G:559:SER:HA	1:G:630:PHE:O	2.16	0.46
1:M:218:LEU:H	1:M:303:GLN:HE21	1.62	0.46
1:J:421:HIS:HB2	1:K:3:LEU:HB3	1.97	0.46
1:J:323:VAL:HG23	1:J:335:ASN:HA	1.96	0.46
1:N:627:HIS:HB2	1:N:640:GLN:HB2	1.98	0.46
1:Q:339:ASP:C	1:Q:341:SER:H	2.19	0.46
1:K:335:ASN:O	1:K:338:LYS:HB2	2.16	0.46
1:O:621:ASP:OD1	1:O:621:ASP:N	2.46	0.46
1:L:179:VAL:HG21	1:L:270:TRP:CH2	2.50	0.46
1:L:146:LEU:HB2	1:L:271:TRP:CD1	2.49	0.46
1:L:145:GLU:HG3	1:L:213:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:ASN:HD21	1:L:209:GLY:HA3	1.81	0.46
1:B:71:ILE:HG21	1:B:154:THR:HG23	1.98	0.46
1:H:258:ALA:HB2	1:H:314:VAL:CG2	2.46	0.46
1:K:34:GLY:C	1:K:499:ILE:HA	2.36	0.46
1:A:169:VAL:HG22	1:A:171:PRO:O	2.15	0.46
1:A:168:ARG:NH1	1:A:241:GLU:OE2	2.49	0.46
1:H:478:ARG:NH2	1:H:478:ARG:CG	2.70	0.46
1:D:506:VAL:O	1:D:507:ASN:C	2.53	0.46
1:K:123:SER:CB	2:K:701:SAH:HN62	2.17	0.46
1:E:143:ASP:O	1:E:146:LEU:HA	2.16	0.46
1:I:478:ARG:NH2	1:I:478:ARG:HG2	2.30	0.46
1:P:253:VAL:HG23	1:P:253:VAL:O	2.15	0.46
1:F:480:GLU:HA	1:F:481:PRO:C	2.35	0.46
1:Q:139:ALA:O	1:Q:142:PHE:HE1	1.99	0.46
1:P:216:VAL:HG22	1:P:218:LEU:HD23	1.98	0.46
1:J:502:ASP:OD2	1:J:616:THR:HG21	2.16	0.46
1:D:452:SER:O	1:D:453:ALA:C	2.54	0.46
1:C:631:ASP:C	1:C:631:ASP:OD1	2.54	0.46
1:C:190:ASN:ND2	1:C:209:GLY:HA3	2.31	0.46
1:G:502:ASP:OD2	1:G:616:THR:HG21	2.16	0.46
1:B:156:LYS:HE2	1:B:246:ILE:O	2.16	0.46
1:A:175:ASN:ND2	1:A:237:LYS:HG2	2.30	0.46
1:N:385:THR:HA	1:N:445:LEU:O	2.15	0.46
1:M:280:THR:CG2	1:M:281:THR:N	2.79	0.46
1:Q:42:ARG:HE	1:Q:43:ASN:ND2	2.14	0.46
1:J:274:ASP:OD2	1:J:277:ARG:CA	2.63	0.46
1:C:314:VAL:HG23	1:C:320:PHE:CD2	2.50	0.46
1:I:379:LYS:CA	1:I:399:THR:HG23	2.36	0.46
1:M:218:LEU:N	1:M:303:GLN:NE2	2.64	0.46
1:M:67:HIS:HD2	1:M:133:ARG:O	1.98	0.46
1:P:73:THR:O	2:P:701:SAH:HA	2.15	0.46
1:G:93:LEU:CD2	1:G:119:ILE:HB	2.46	0.46
1:N:327:ASP:OD1	1:N:328:GLU:N	2.49	0.46
1:C:16:VAL:HG22	4:C:811:HOH:O	2.16	0.46
1:A:272:ASP:C	1:A:272:ASP:OD1	2.54	0.46
1:A:145:GLU:O	1:A:146:LEU:HB3	2.16	0.46
1:G:151:ALA:O	1:G:155:PHE:HD2	1.99	0.46
1:F:7:ASN:ND2	1:F:640:GLN:OE1	2.45	0.46
1:I:492:LYS:HA	1:I:573:ASN:OD1	2.16	0.46
1:E:42:ARG:HE	1:E:43:ASN:HD21	1.64	0.46
1:F:203:PRO:HA	1:F:422:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:THR:HA	1:E:445:LEU:O	2.16	0.46
1:G:190:ASN:ND2	1:G:209:GLY:HA3	2.31	0.46
1:D:626:LEU:CD2	1:D:628:ALA:HB2	2.45	0.46
1:I:298:ARG:O	1:I:301:TRP:O	2.34	0.46
1:K:257:VAL:O	1:K:257:VAL:HG12	2.14	0.46
1:G:156:LYS:HA	1:G:243:GLU:HB3	1.97	0.46
1:H:67:HIS:CE1	1:H:89:LYS:HE3	2.51	0.46
1:H:242:HIS:O	1:H:245:LYS:HB2	2.16	0.46
1:M:364:MET:HG3	1:M:370:PHE:CE2	2.51	0.46
1:P:406:ILE:HD13	1:P:434:VAL:HA	1.97	0.46
1:A:554:ASP:O	1:A:555:GLY:O	2.34	0.46
1:C:140:GLU:CG	1:C:140:GLU:O	2.61	0.46
1:F:73:THR:O	1:F:76:GLY:N	2.49	0.46
1:G:35:ASP:OD1	1:G:35:ASP:N	2.48	0.46
1:H:239:ASP:OD1	1:H:242:HIS:HB2	2.16	0.46
1:H:460:LEU:HD21	1:H:579:MET:CE	2.46	0.46
1:P:502:ASP:OD2	1:P:616:THR:HB	2.15	0.46
1:M:418:LYS:HB2	1:M:418:LYS:HE3	1.79	0.46
1:K:367:ASN:OD1	1:K:370:PHE:N	2.48	0.46
1:H:133:ARG:HG3	1:H:164:LYS:HG2	1.98	0.46
1:J:216:VAL:O	1:J:302:MET:HG2	2.16	0.46
1:F:48:ALA:O	1:F:51:LYS:N	2.48	0.46
1:D:138:VAL:HG23	1:D:170:VAL:HB	1.97	0.46
1:M:289:TRP:O	1:M:290:LYS:HG2	2.16	0.46
1:Q:99:MET:O	1:Q:102:CYS:HB3	2.16	0.45
1:R:353:LEU:HD22	1:R:357:THR:CG2	2.46	0.45
1:D:45:LYS:O	1:D:275:MET:HG2	2.15	0.45
1:M:483:MET:CE	1:M:550:ARG:HG2	2.46	0.45
1:R:316:MET:HA	1:R:317:ASN:HA	1.69	0.45
1:R:243:GLU:N	1:R:243:GLU:OE1	2.43	0.45
1:P:164:LYS:O	1:P:167:CYS:HB2	2.16	0.45
1:O:412:PHE:HE2	1:O:451:MET:HG2	1.81	0.45
1:K:404:THR:HG23	1:K:429:GLU:HG3	1.99	0.45
1:C:61:ASN:N	1:C:61:ASN:HD22	2.14	0.45
1:K:360:HIS:HB2	1:K:606:GLY:HA3	1.98	0.45
1:J:291:ASN:HB3	1:J:295:TYR:HB2	1.98	0.45
1:L:353:LEU:HD22	1:L:357:THR:HG21	1.97	0.45
1:G:217:GLN:HB2	1:G:536:GLU:HB3	1.98	0.45
1:C:247:ILE:HB	1:C:250:GLU:OE2	2.16	0.45
1:G:489:ILE:HG12	1:G:541:VAL:HG22	1.99	0.45
1:B:569:MET:HA	1:B:572:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:218:LEU:HD23	1:Q:218:LEU:HA	1.42	0.45
1:E:490:PRO:CB	1:E:569:MET:HE1	2.46	0.45
1:N:566:ILE:HG21	1:N:569:MET:CE	2.42	0.45
1:F:502:ASP:OD2	1:F:616:THR:HG21	2.17	0.45
1:J:218:LEU:N	1:J:303:GLN:NE2	2.62	0.45
1:G:478:ARG:CG	1:G:478:ARG:HH21	2.29	0.45
1:K:179:VAL:CG2	1:K:270:TRP:CH2	2.99	0.45
1:J:144:THR:CG2	1:J:144:THR:O	2.64	0.45
1:Q:287:PRO:HG2	1:Q:289:TRP:CZ2	2.50	0.45
1:Q:468:VAL:O	1:Q:472:MET:HG3	2.16	0.45
1:K:193:PRO:HA	1:K:362:ASN:HD21	1.82	0.45
1:B:466:VAL:HG11	1:B:553:ILE:CG2	2.46	0.45
1:P:39:ASP:OD2	1:P:298:ARG:HD3	2.16	0.45
1:O:427:ASN:OD1	1:O:427:ASN:N	2.49	0.45
1:A:84:ARG:HG3	1:A:112:TRP:CZ2	2.50	0.45
1:L:447:GLU:N	1:L:448:PRO:HA	2.32	0.45
1:E:48:ALA:HA	1:E:51:LYS:HB2	1.98	0.45
1:Q:395:LEU:C	1:Q:397:ALA:H	2.18	0.45
1:A:385:THR:HA	1:A:445:LEU:O	2.16	0.45
1:O:143:ASP:HB3	1:O:149:GLU:HG3	1.98	0.45
1:B:297:TRP:CE3	1:B:495:ASP:HB3	2.51	0.45
1:F:72:GLY:CA	2:F:701:SAH:O4'	2.65	0.45
1:H:269:MET:CG	1:H:306:TYR:HE1	2.27	0.45
1:M:35:ASP:HB3	1:M:300:HIS:H	1.80	0.45
1:H:47:LEU:HD22	1:H:51:LYS:CD	2.46	0.45
1:N:315:GLU:CB	1:N:318:GLN:HG2	2.44	0.45
1:P:110:SER:HB2	1:P:112:TRP:CZ3	2.51	0.45
1:G:540:ILE:HB	1:G:599:GLY:O	2.15	0.45
1:A:447:GLU:H	1:A:448:PRO:HA	1.82	0.45
1:O:460:LEU:HD11	1:O:637:ILE:HD11	1.98	0.45
1:C:456:PRO:HD2	1:C:457:TRP:CE3	2.51	0.45
1:B:190:ASN:O	1:B:190:ASN:ND2	2.50	0.45
1:B:119:ILE:HG22	1:B:121:GLU:HG2	1.99	0.45
1:L:157:GLU:HA	1:L:160:GLU:HG2	1.97	0.45
1:C:592:LEU:HD21	1:C:595:ILE:HD11	1.97	0.45
1:K:292:LYS:HA	1:K:293:ASN:HB3	1.98	0.45
1:M:174:GLY:HA2	1:M:273:ILE:HA	1.98	0.45
1:B:357:THR:O	1:B:361:VAL:HG23	2.16	0.45
1:B:43:ASN:O	1:B:81:MET:HE1	2.16	0.45
1:L:137:ILE:HB	1:L:169:VAL:HB	1.97	0.45
1:A:480:GLU:HG2	1:A:584:GLY:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:VAL:O	1:K:265:ASP:N	2.49	0.45
1:I:420:ILE:HD11	1:I:428:VAL:CG2	2.46	0.45
1:B:534:LEU:HD11	1:B:611:VAL:CG1	2.46	0.45
1:M:385:THR:HG22	4:M:802:HOH:O	2.15	0.45
1:B:535:TRP:CG	1:B:605:LYS:HG2	2.51	0.45
1:G:258:ALA:CB	1:G:314:VAL:HG13	2.47	0.45
1:N:287:PRO:O	1:N:291:ASN:HB3	2.16	0.45
1:F:214:PHE:O	1:F:304:ALA:HA	2.17	0.45
1:B:287:PRO:O	1:B:289:TRP:N	2.50	0.45
1:A:4:GLU:OE2	1:A:13:ARG:NH1	2.50	0.45
1:F:179:VAL:HG22	1:F:232:PRO:HA	1.98	0.45
1:I:72:GLY:O	2:I:701:SAH:N	2.50	0.45
1:M:42:ARG:HH11	1:M:140:GLU:CG	2.20	0.45
1:Q:480:GLU:HA	1:Q:481:PRO:C	2.36	0.45
1:P:258:ALA:O	1:P:317:ASN:HA	2.17	0.45
1:E:83:ALA:O	1:E:84:ARG:C	2.55	0.45
1:O:567:ASP:O	1:O:568:ASN:CB	2.62	0.45
1:J:45:LYS:O	1:J:275:MET:HG3	2.17	0.45
1:M:67:HIS:N	1:M:135:ASP:OD2	2.36	0.45
1:B:56:GLU:O	1:B:59:HIS:HB2	2.17	0.45
1:B:193:PRO:HA	1:B:362:ASN:ND2	2.32	0.45
1:A:488:ALA:HA	1:A:576:PRO:O	2.16	0.45
1:C:349:LEU:HD11	1:C:391:PHE:HZ	1.82	0.45
1:I:111:PRO:HB2	1:I:112:TRP:CE3	2.52	0.45
1:N:577:MET:CE	1:N:626:LEU:HD11	2.47	0.45
1:I:612:TYR:CZ	1:I:614:PRO:HA	2.51	0.45
1:J:597:SER:HB2	1:J:598:ALA:HB3	1.91	0.45
1:E:241:GLU:HG3	1:E:277:ARG:NH2	2.31	0.45
1:D:550:ARG:H	1:D:560:GLN:NE2	2.11	0.45
1:K:188:MET:O	1:K:359:TYR:HA	2.16	0.45
1:Q:35:ASP:O	1:Q:36:MET:C	2.53	0.45
1:E:443:ILE:HG12	1:E:445:LEU:HD13	1.99	0.45
1:E:275:MET:CE	1:E:283:ILE:HG13	2.46	0.45
1:B:567:ASP:O	1:B:568:ASN:CB	2.64	0.45
1:E:161:ARG:HB3	1:E:162:LEU:CD1	2.46	0.45
1:O:470:LYS:HE3	1:O:554:ASP:HA	1.98	0.45
1:E:452:SER:O	1:E:453:ALA:C	2.54	0.45
1:F:269:MET:HE3	1:F:304:ALA:HB3	1.99	0.45
1:C:349:LEU:HD12	1:C:415:ILE:HD13	1.99	0.45
1:L:216:VAL:O	1:L:302:MET:HG2	2.17	0.45
1:F:95:VAL:HG23	1:F:122:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:ASP:OD2	1:M:65:LYS:HB2	2.16	0.45
1:M:432:GLU:HG2	1:M:433:LYS:HG3	1.98	0.45
1:K:203:PRO:HA	1:K:422:TYR:CG	2.52	0.45
1:Q:68:VAL:HG23	1:Q:136:ILE:HB	1.99	0.45
1:Q:68:VAL:HG13	1:Q:90:VAL:HG12	1.90	0.45
1:E:258:ALA:CB	1:E:314:VAL:HG13	2.47	0.45
1:N:146:LEU:HB2	1:N:271:TRP:CD1	2.52	0.45
1:P:368:GLN:O	1:P:369:LYS:C	2.55	0.45
1:M:169:VAL:HG22	1:M:171:PRO:O	2.16	0.45
1:M:485:VAL:HG12	1:M:580:GLU:HB2	1.98	0.45
1:K:491:GLU:OE1	1:K:539:GLY:HA3	2.16	0.45
1:P:168:ARG:HB3	1:P:168:ARG:HE	1.67	0.45
1:C:323:VAL:HG12	1:C:325:ASN:ND2	2.31	0.45
1:H:258:ALA:HB2	1:H:314:VAL:HG22	1.97	0.45
1:A:84:ARG:O	1:A:85:GLU:HB2	2.17	0.45
1:H:56:GLU:O	1:H:60:GLU:HG2	2.17	0.45
1:B:292:LYS:HA	1:B:293:ASN:HA	1.75	0.45
1:Q:437:LEU:HA	1:Q:437:LEU:HD23	1.87	0.45
1:O:277:ARG:HG2	1:O:277:ARG:O	2.17	0.45
1:J:199:LYS:HA	1:J:200:ASP:HA	1.71	0.45
1:N:268:LEU:HD12	1:N:289:TRP:HH2	1.82	0.45
1:A:104:ARG:HA	1:A:107:THR:HG22	1.99	0.45
1:P:241:GLU:HG3	1:P:277:ARG:NH2	2.10	0.45
1:M:447:GLU:HB2	1:M:449:PHE:N	2.32	0.45
1:M:379:LYS:CA	1:M:399:THR:HG23	2.38	0.45
1:F:275:MET:HE1	1:F:283:ILE:CG1	2.39	0.45
1:Q:321:GLU:O	1:Q:322:ILE:HD12	2.17	0.45
1:B:412:PHE:CE2	1:B:451:MET:HG2	2.44	0.45
1:N:549:LEU:HD21	1:N:628:ALA:HB1	1.98	0.45
1:H:61:ASN:O	1:H:62:THR:C	2.55	0.45
1:Q:95:VAL:CB	1:Q:122:ARG:HG3	2.46	0.45
1:K:373:GLU:O	1:K:377:LEU:HD12	2.17	0.45
1:N:297:TRP:CD2	1:N:495:ASP:HB3	2.52	0.45
1:R:344:TYR:O	1:R:346:VAL:HG13	2.17	0.45
1:L:16:VAL:CG1	1:L:17:VAL:N	2.79	0.45
1:F:158:ALA:HA	1:F:162:LEU:HB2	1.98	0.45
1:L:629:LEU:O	1:L:637:ILE:HA	2.17	0.45
1:Q:466:VAL:CG1	1:Q:470:LYS:HE2	2.46	0.45
1:Q:381:LEU:O	1:Q:400:ALA:HB1	2.17	0.45
1:A:178:ILE:HA	1:A:268:LEU:O	2.17	0.45
1:Q:316:MET:HA	1:Q:317:ASN:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:ARG:NH1	1:K:168:ARG:HG2	2.32	0.45
1:M:450:TYR:HE1	1:M:462:PHE:HB2	1.82	0.45
1:P:317:ASN:HD22	1:P:317:ASN:C	2.16	0.45
1:E:84:ARG:NH1	1:E:509:PHE:CE2	2.85	0.45
1:M:382:HIS:HD2	1:M:402:ARG:HG3	1.80	0.45
1:M:542:LYS:CG	1:M:571:SER:HB2	2.46	0.45
1:M:141:VAL:CG1	1:M:141:VAL:O	2.65	0.45
1:O:292:LYS:HD2	1:O:292:LYS:HA	1.54	0.45
1:J:534:LEU:HG	1:J:609:GLN:HB2	1.98	0.45
1:I:200:ASP:OD1	1:I:200:ASP:N	2.39	0.45
1:F:20:GLU:H	1:F:20:GLU:HG3	1.62	0.45
1:O:19:GLU:HG2	1:O:19:GLU:O	2.14	0.45
1:K:176:VAL:HG22	1:K:235:ALA:HB3	1.99	0.45
1:N:414:ASP:O	1:N:418:LYS:HG3	2.17	0.45
1:N:178:ILE:HG13	1:N:233:ILE:HB	1.99	0.45
1:M:95:VAL:HG13	1:M:96:PHE:H	1.80	0.45
1:K:143:ASP:O	1:K:145:GLU:N	2.50	0.45
1:M:493:PHE:HA	1:M:539:GLY:CA	2.47	0.45
1:J:414:ASP:OD2	1:K:19:GLU:HG2	2.17	0.45
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.17	0.45
1:Q:631:ASP:HB3	1:Q:634:THR:OG1	2.16	0.45
1:Q:431:ILE:HD12	1:Q:436:SER:HB2	1.99	0.45
1:O:72:GLY:N	1:O:93:LEU:O	2.48	0.45
1:F:325:ASN:HB3	1:F:332:TRP:CE2	2.52	0.45
1:M:632:LYS:HG3	1:M:633:SER:N	2.32	0.45
1:B:157:GLU:HA	1:B:160:GLU:HG2	1.98	0.45
1:M:569:MET:CG	1:M:624:LEU:HD11	2.39	0.44
1:N:54:ILE:HG13	1:N:58:LYS:HD3	1.99	0.44
1:Q:480:GLU:CG	1:Q:584:GLY:N	2.78	0.44
1:P:365:PHE:O	1:P:371:LYS:NZ	2.50	0.44
1:J:600:VAL:HA	1:J:601:PRO:HD3	1.86	0.44
1:R:505:THR:HA	1:R:509:PHE:O	2.17	0.44
1:B:123:SER:C	1:B:125:ASP:H	2.18	0.44
1:P:26:GLN:O	1:P:30:ARG:HD2	2.17	0.44
1:P:136:ILE:HA	1:P:168:ARG:O	2.16	0.44
1:I:181:VAL:HG21	1:I:226:PHE:HB2	1.98	0.44
1:R:476:GLU:CD	1:R:476:GLU:H	2.20	0.44
1:B:427:ASN:HA	1:C:8:GLN:HE22	1.81	0.44
1:O:480:GLU:HG3	1:O:481:PRO:HA	1.99	0.44
1:G:420:ILE:HD11	1:G:428:VAL:HG22	1.99	0.44
1:O:512:SER:O	1:O:515:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:GLU:HG2	1:E:433:LYS:HG2	1.99	0.44
1:M:276:ASP:OD1	1:M:278:ASN:HB2	2.16	0.44
1:O:623:SER:O	1:O:624:LEU:HB3	2.17	0.44
1:L:631:ASP:OD1	1:L:633:SER:N	2.47	0.44
1:D:218:LEU:H	1:D:303:GLN:NE2	2.15	0.44
1:O:353:LEU:HD22	1:O:357:THR:HG21	1.98	0.44
1:O:541:VAL:N	1:O:599:GLY:O	2.41	0.44
1:L:228:GLU:OE2	1:L:290:LYS:HE2	2.17	0.44
1:M:316:MET:HA	1:M:317:ASN:HA	1.78	0.44
1:M:231:GLU:HG2	1:M:231:GLU:H	1.58	0.44
1:O:483:MET:CG	1:O:550:ARG:HH21	2.30	0.44
1:F:319:THR:O	1:F:320:PHE:HB3	2.17	0.44
1:H:632:LYS:HG2	1:H:633:SER:N	2.31	0.44
1:A:67:HIS:CE1	1:A:91:THR:HG23	2.47	0.44
1:K:378:SER:HB2	1:K:399:THR:HG22	1.99	0.44
1:G:450:TYR:H	1:G:459:HIS:CD2	2.22	0.44
1:J:300:HIS:HE1	1:J:301:TRP:CE3	2.35	0.44
1:N:460:LEU:HB3	1:N:463:LEU:HD22	1.99	0.44
1:Q:569:MET:CE	1:Q:575:ILE:HG12	2.47	0.44
1:C:447:GLU:N	1:C:448:PRO:HA	2.33	0.44
1:P:48:ALA:HA	1:P:51:LYS:HD2	1.99	0.44
1:E:492:LYS:HB2	1:E:542:LYS:HE2	1.99	0.44
1:M:287:PRO:O	1:M:288:LYS:C	2.56	0.44
1:P:42:ARG:NH2	1:P:43:ASN:HD21	2.09	0.44
1:M:68:VAL:HA	1:M:136:ILE:O	2.17	0.44
1:K:169:VAL:CG1	1:K:241:GLU:HG2	2.39	0.44
1:R:379:LYS:CA	1:R:399:THR:HG21	2.42	0.44
1:K:375:ASP:O	1:K:399:THR:HG21	2.17	0.44
1:J:300:HIS:CE1	1:J:301:TRP:CE3	3.05	0.44
1:Q:583:PHE:CB	1:Q:588:LEU:CD1	2.96	0.44
1:F:159:LEU:HB3	1:F:243:GLU:HG2	1.98	0.44
1:H:190:ASN:ND2	1:H:209:GLY:HA3	2.31	0.44
1:G:385:THR:CG2	1:G:405:ILE:HG23	2.47	0.44
1:N:353:LEU:HB3	1:N:357:THR:HB	1.99	0.44
1:P:26:GLN:O	1:P:30:ARG:HD3	2.16	0.44
1:O:145:GLU:HA	1:O:269:MET:HE1	2.00	0.44
1:G:67:HIS:HE1	1:G:91:THR:HG23	1.81	0.44
1:I:452:SER:O	1:I:453:ALA:C	2.56	0.44
1:O:395:LEU:HA	1:O:395:LEU:HD23	1.75	0.44
1:E:20:GLU:HG3	1:E:20:GLU:H	1.21	0.44
1:I:507:ASN:N	1:I:507:ASN:ND2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:516:GLU:O	1:L:520:LYS:HG3	2.18	0.44
1:I:190:ASN:CG	1:I:190:ASN:O	2.56	0.44
1:J:178:ILE:HB	1:J:267:LEU:HD22	1.99	0.44
1:R:192:ILE:HG23	1:R:204:LEU:HD12	1.99	0.44
1:E:488:ALA:HB2	1:E:577:MET:HE3	1.98	0.44
1:B:519:THR:O	1:B:520:LYS:C	2.54	0.44
1:Q:216:VAL:HG13	1:Q:218:LEU:HG	2.00	0.44
1:N:387:GLY:HA2	1:N:450:TYR:CZ	2.53	0.44
1:N:460:LEU:C	1:N:462:PHE:N	2.70	0.44
1:N:218:LEU:HD12	1:N:303:GLN:CB	2.47	0.44
1:Q:460:LEU:C	1:Q:462:PHE:N	2.71	0.44
1:M:269:MET:HG2	1:M:306:TYR:CE2	2.51	0.44
1:M:502:ASP:OD1	1:M:616:THR:HG21	2.17	0.44
1:L:143:ASP:O	1:L:146:LEU:N	2.43	0.44
1:F:51:LYS:HG3	1:F:85:GLU:HG3	1.98	0.44
1:O:550:ARG:HD2	1:O:550:ARG:HA	1.80	0.44
1:I:31:SER:O	1:I:33:PHE:CD2	2.71	0.44
1:G:28:LEU:HG	1:G:28:LEU:O	2.17	0.44
1:M:80:LEU:HD21	1:M:107:THR:HG22	2.00	0.44
1:I:156:LYS:NZ	1:I:243:GLU:O	2.51	0.44
1:Q:375:ASP:CA	1:Q:399:THR:HG21	2.21	0.44
1:N:168:ARG:NH1	1:N:241:GLU:OE2	2.51	0.44
1:B:43:ASN:N	1:B:43:ASN:HD22	2.07	0.44
1:D:50:LEU:O	1:D:54:ILE:CG1	2.65	0.44
1:M:269:MET:HG3	1:M:304:ALA:HB3	2.00	0.44
1:G:403:VAL:HB	1:G:428:VAL:HB	1.99	0.44
1:M:316:MET:O	1:M:316:MET:HG3	2.17	0.44
1:Q:404:THR:HG23	1:Q:429:GLU:HG3	2.00	0.44
1:F:392:LEU:HD22	1:F:392:LEU:O	2.17	0.44
1:E:362:ASN:O	1:E:366:GLU:HG2	2.18	0.44
1:Q:108:SER:HA	1:Q:113:SER:HB2	1.99	0.44
1:Q:490:PRO:HB2	1:Q:572:SER:OG	2.18	0.44
1:I:51:LYS:HG3	1:I:85:GLU:HG2	2.00	0.44
1:J:56:GLU:OE1	1:J:168:ARG:HD2	2.18	0.44
1:D:140:GLU:C	1:D:140:GLU:OE1	2.56	0.44
1:Q:235:ALA:HB1	1:Q:324:CYS:SG	2.58	0.44
1:P:497:GLN:H	1:P:497:GLN:HE21	1.65	0.44
1:Q:566:ILE:HG22	1:Q:569:MET:HE2	2.00	0.44
1:F:277:ARG:O	1:F:279:GLY:N	2.51	0.44
1:N:201:GLU:HA	1:N:422:TYR:OH	2.17	0.44
1:L:359:TYR:C	1:L:359:TYR:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:LEU:O	1:I:185:LEU:HD22	2.18	0.44
1:J:449:PHE:C	1:J:449:PHE:CD1	2.91	0.44
1:R:94:GLU:OE2	2:R:701:SAH:H1'	2.18	0.44
1:H:211:ALA:HB2	1:H:343:SER:O	2.17	0.44
1:A:412:PHE:HE2	1:A:451:MET:HG2	1.82	0.44
1:J:395:LEU:O	1:J:398:LYS:HB2	2.18	0.44
1:Q:383:VAL:HG23	1:Q:384:ALA:N	2.33	0.44
1:Q:52:THR:O	1:Q:55:ALA:HB3	2.17	0.44
1:B:489:ILE:HD13	1:B:541:VAL:HG22	1.99	0.44
1:J:490:PRO:HB3	1:J:569:MET:HE2	1.81	0.44
1:Q:168:ARG:NH1	1:Q:168:ARG:CG	2.65	0.44
1:R:201:GLU:C	1:R:203:PRO:HD3	2.37	0.44
1:A:434:VAL:HG13	1:A:469:LEU:CD1	2.47	0.44
1:O:233:ILE:CD1	1:O:254:ARG:HB3	2.42	0.44
1:P:84:ARG:O	1:P:85:GLU:HB2	2.18	0.44
1:R:69:LEU:HD13	1:R:91:THR:HG23	1.99	0.44
1:P:110:SER:O	1:P:113:SER:HB3	2.18	0.44
1:I:145:GLU:HG3	1:I:331:LEU:HD22	2.00	0.44
1:C:57:LYS:HG2	1:C:135:ASP:HB3	1.99	0.44
1:O:145:GLU:HA	1:O:269:MET:CE	2.48	0.44
1:M:383:VAL:HG13	1:M:403:VAL:HG22	2.00	0.44
1:F:264:ILE:HB	1:F:312:LYS:HB3	2.00	0.44
1:J:593:LEU:HD12	1:J:593:LEU:HA	1.91	0.44
1:K:244:GLU:H	1:K:244:GLU:CD	2.19	0.44
1:Q:146:LEU:HD13	1:Q:271:TRP:CD2	2.53	0.44
1:F:186:LEU:O	1:F:307:TYR:OH	2.21	0.44
1:A:103:ALA:O	1:A:107:THR:CB	2.47	0.44
1:Q:169:VAL:HG22	1:Q:241:GLU:HG2	2.00	0.44
1:R:550:ARG:HB2	1:R:550:ARG:CZ	2.47	0.44
1:M:68:VAL:HB	1:M:90:VAL:HG22	2.00	0.44
1:G:107:THR:O	1:G:110:SER:OG	2.35	0.44
1:G:42:ARG:HG3	1:G:301:TRP:CH2	2.53	0.44
1:K:147:ILE:HD11	1:K:331:LEU:HD13	2.00	0.44
1:R:168:ARG:HG2	1:R:241:GLU:OE1	2.18	0.44
1:M:269:MET:CG	1:M:304:ALA:HB3	2.48	0.44
1:O:297:TRP:CE3	1:O:495:ASP:HB3	2.52	0.44
1:R:67:HIS:CE1	1:R:89:LYS:HG2	2.53	0.44
1:L:80:LEU:HB3	1:L:509:PHE:CE1	2.53	0.44
1:F:292:LYS:HA	1:F:292:LYS:HD2	1.74	0.44
1:M:235:ALA:HA	1:M:254:ARG:HG3	2.00	0.44
1:D:297:TRP:CE3	1:D:495:ASP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLU:O	1:B:233:ILE:HG22	2.18	0.44
1:J:191:ASP:OD2	1:J:194:ARG:NH1	2.51	0.43
1:F:625:CYS:HB2	1:F:644:SER:HA	2.00	0.43
1:G:497:GLN:N	1:G:497:GLN:NE2	2.60	0.43
1:Q:274:ASP:OD2	1:Q:277:ARG:N	2.50	0.43
1:O:442:ASP:O	1:O:478:ARG:CB	2.62	0.43
1:B:169:VAL:HG22	1:B:171:PRO:O	2.17	0.43
1:C:338:LYS:N	1:F:244:GLU:HG3	2.32	0.43
1:I:63:ASP:N	1:I:63:ASP:OD1	2.48	0.43
1:K:510:ASP:C	1:K:512:SER:H	2.22	0.43
1:Q:513:PHE:O	1:Q:516:GLU:HB3	2.18	0.43
1:E:480:GLU:OE2	1:E:482:HIS:CD2	2.69	0.43
1:C:275:MET:HE1	1:C:283:ILE:H	1.82	0.43
1:R:35:ASP:OD1	1:R:300:HIS:N	2.47	0.43
1:O:451:MET:HG3	1:O:452:SER:N	2.32	0.43
1:O:219:SER:HB3	1:O:288:LYS:HB2	2.00	0.43
1:O:404:THR:HG21	1:O:437:LEU:HD23	2.00	0.43
1:E:63:ASP:CG	1:E:64:GLY:H	2.21	0.43
1:K:171:PRO:HB3	1:K:275:MET:HE1	1.99	0.43
1:B:168:ARG:HG2	1:B:168:ARG:NH1	2.31	0.43
1:N:258:ALA:HB3	1:N:315:GLU:O	2.18	0.43
1:D:518:SER:O	1:D:522:ARG:HG3	2.18	0.43
1:R:178:ILE:HA	1:R:268:LEU:O	2.18	0.43
1:O:414:ASP:O	1:O:418:LYS:HG3	2.17	0.43
1:C:288:LYS:HG3	1:C:295:TYR:CE2	2.53	0.43
1:N:251:SER:OG	1:N:340:LYS:HD3	2.18	0.43
1:J:54:ILE:HD13	1:J:85:GLU:HB3	1.99	0.43
1:C:146:LEU:HD13	1:C:271:TRP:CG	2.53	0.43
1:L:190:ASN:ND2	1:L:209:GLY:HA3	2.33	0.43
1:C:578:TRP:CB	1:C:591:GLY:HA3	2.48	0.43
1:Q:67:HIS:O	1:Q:135:ASP:N	2.47	0.43
1:C:230:SER:OG	1:C:231:GLU:O	2.36	0.43
1:K:348:GLY:CA	1:K:411:ARG:HH22	2.31	0.43
1:C:403:VAL:HB	1:C:428:VAL:HB	2.00	0.43
1:P:156:LYS:O	1:P:160:GLU:CG	2.65	0.43
1:J:194:ARG:HG2	1:J:201:GLU:CB	2.37	0.43
1:B:218:LEU:HD22	1:B:221:MET:CE	2.48	0.43
1:E:623:SER:O	1:E:624:LEU:HD23	2.18	0.43
1:R:218:LEU:HA	1:R:218:LEU:HD23	1.72	0.43
1:O:548:ILE:HD12	1:O:626:LEU:HD13	2.01	0.43
1:R:485:VAL:HA	1:R:549:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:GLU:O	1:O:201:GLU:HB2	2.17	0.43
1:M:349:LEU:HD11	1:M:353:LEU:HD12	1.99	0.43
1:P:83:ALA:HB1	1:P:112:TRP:CG	2.53	0.43
1:L:84:ARG:HG3	1:L:112:TRP:HZ2	1.83	0.43
1:H:70:ASP:HA	1:H:138:VAL:O	2.18	0.43
1:N:339:ASP:OD1	1:N:340:LYS:N	2.51	0.43
1:B:514:PHE:HA	1:B:517:ILE:HG12	1.99	0.43
1:I:451:MET:HE2	1:I:452:SER:HA	1.99	0.43
1:Q:67:HIS:HA	1:Q:89:LYS:O	2.17	0.43
1:K:229:LEU:CD1	1:K:314:VAL:HG12	2.48	0.43
1:R:512:SER:O	1:R:515:ASP:HB2	2.18	0.43
1:J:124:THR:O	1:J:161:ARG:NH2	2.51	0.43
1:N:474:GLY:HA3	1:N:476:GLU:OE2	2.18	0.43
1:L:141:VAL:CG1	1:L:141:VAL:O	2.66	0.43
1:K:641:PHE:CD1	1:K:641:PHE:N	2.85	0.43
1:I:593:LEU:HD12	1:I:593:LEU:HA	1.73	0.43
1:F:178:ILE:HB	1:F:267:LEU:HD22	1.99	0.43
1:N:447:GLU:N	1:N:448:PRO:HA	2.32	0.43
1:H:455:ASN:HB3	1:H:457:TRP:CE2	2.53	0.43
1:Q:140:GLU:O	1:Q:140:GLU:HG3	2.17	0.43
1:D:622:LYS:CD	1:D:622:LYS:N	2.79	0.43
1:R:52:THR:HG21	1:R:276:ASP:CB	2.46	0.43
1:R:69:LEU:HD12	1:R:69:LEU:C	2.39	0.43
1:J:93:LEU:HD23	1:J:119:ILE:HB	2.01	0.43
1:B:111:PRO:HG2	1:B:112:TRP:CH2	2.53	0.43
1:R:466:VAL:HG11	1:R:553:ILE:HG21	2.00	0.43
1:O:483:MET:HB3	1:O:582:GLU:HG2	1.99	0.43
1:N:190:ASN:HD21	1:N:209:GLY:HA3	1.83	0.43
1:O:367:ASN:O	1:O:371:LYS:HD3	2.18	0.43
1:O:466:VAL:HA	1:O:469:LEU:HB2	1.99	0.43
1:A:297:TRP:CE3	1:A:495:ASP:HB3	2.53	0.43
1:J:226:PHE:CZ	1:J:289:TRP:CZ2	3.06	0.43
1:E:643:LYS:O	1:E:644:SER:OG	2.27	0.43
1:J:68:VAL:O	1:J:90:VAL:HA	2.18	0.43
1:O:178:ILE:HG21	1:O:333:PHE:CZ	2.53	0.43
1:J:261:SER:OG	1:J:316:MET:N	2.52	0.43
1:N:55:ALA:CA	1:N:58:LYS:HD2	2.47	0.43
1:R:487:LYS:HE3	1:R:547:GLU:HG2	2.00	0.43
1:M:111:PRO:C	1:M:113:SER:N	2.72	0.43
1:M:480:GLU:CG	1:M:584:GLY:H	2.32	0.43
1:A:144:THR:O	1:A:269:MET:HE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ARG:HG3	1:G:301:TRP:CZ3	2.53	0.43
1:K:534:LEU:C	1:K:536:GLU:H	2.22	0.43
1:Q:143:ASP:C	1:Q:145:GLU:N	2.71	0.43
1:R:136:ILE:HG23	1:R:168:ARG:O	2.18	0.43
1:F:368:GLN:NE2	1:F:371:LYS:CE	2.80	0.43
1:F:143:ASP:O	1:F:146:LEU:N	2.34	0.43
1:P:600:VAL:HA	1:P:601:PRO:HD3	1.86	0.43
1:B:388:GLU:OE1	1:B:452:SER:HB2	2.19	0.43
1:H:375:ASP:O	1:H:399:THR:HG21	2.19	0.43
1:J:290:LYS:HD3	1:J:290:LYS:HA	1.92	0.43
1:A:359:TYR:CD1	1:A:359:TYR:C	2.92	0.43
1:K:492:LYS:HD3	1:K:542:LYS:NZ	2.33	0.43
1:Q:1:MET:O	1:Q:17:VAL:HG12	2.19	0.43
1:N:612:TYR:CE2	1:N:614:PRO:HA	2.53	0.43
1:G:378:SER:O	1:G:400:ALA:HA	2.18	0.43
1:L:569:MET:HA	1:L:572:SER:HB2	2.00	0.43
1:H:449:PHE:HA	1:H:459:HIS:CD2	2.54	0.43
1:K:550:ARG:O	1:K:560:GLN:OE1	2.36	0.43
1:M:4:GLU:O	1:O:420:ILE:HD11	2.19	0.43
1:I:550:ARG:HH11	1:I:550:ARG:CG	2.30	0.43
1:R:297:TRP:CZ3	1:R:495:ASP:HB3	2.54	0.43
1:K:616:THR:O	1:K:618:LEU:N	2.52	0.43
1:K:264:ILE:HD12	1:K:312:LYS:HG3	2.01	0.43
1:C:176:VAL:HG13	1:C:236:PHE:HB2	1.99	0.43
1:K:253:VAL:CG2	1:K:253:VAL:O	2.66	0.43
1:M:515:ASP:O	1:M:519:THR:HB	2.18	0.43
1:P:480:GLU:OE2	1:P:482:HIS:HD2	2.01	0.43
1:I:264:ILE:HD12	1:I:312:LYS:HG2	2.00	0.43
1:E:384:ALA:O	1:E:444:VAL:HA	2.18	0.43
1:A:216:VAL:O	1:A:302:MET:HG2	2.18	0.43
1:N:437:LEU:HD11	1:N:441:PRO:HD3	2.00	0.43
1:E:269:MET:HG2	1:E:306:TYR:CE1	2.54	0.43
1:G:489:ILE:CD1	1:G:541:VAL:HG21	2.48	0.43
1:O:7:ASN:HD21	1:O:640:GLN:NE2	2.14	0.43
1:H:480:GLU:HG3	1:H:584:GLY:H	1.84	0.43
1:N:169:VAL:HG12	1:N:241:GLU:HG2	2.00	0.43
1:P:161:ARG:HB3	1:P:162:LEU:HD13	2.01	0.43
1:I:570:SER:CB	1:I:622:LYS:HG2	2.38	0.43
1:C:489:ILE:HG12	1:C:541:VAL:HG22	1.99	0.43
1:M:615:ILE:CG1	1:M:618:LEU:HD22	2.48	0.43
1:A:480:GLU:HG2	1:A:584:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:HG3	1:D:112:TRP:CZ2	2.54	0.43
1:B:476:GLU:N	1:B:476:GLU:CD	2.72	0.43
1:O:269:MET:HG2	1:O:306:TYR:CE1	2.54	0.43
1:P:218:LEU:H	1:P:303:GLN:HE21	1.66	0.43
1:G:427:ASN:HA	1:H:8:GLN:OE1	2.18	0.43
1:N:214:PHE:C	1:N:214:PHE:CD1	2.91	0.43
1:M:151:ALA:O	1:M:154:THR:HG22	2.18	0.43
1:D:47:LEU:HD22	1:D:51:LYS:HE2	2.01	0.43
1:D:190:ASN:ND2	1:D:209:GLY:HA3	2.33	0.43
1:A:460:LEU:HD22	1:A:463:LEU:HD22	2.00	0.43
1:L:69:LEU:HD12	1:L:91:THR:O	2.18	0.43
1:E:54:ILE:HD13	1:E:87:ALA:H	1.83	0.43
1:L:258:ALA:O	1:L:317:ASN:HA	2.18	0.43
1:E:176:VAL:CG1	1:E:236:PHE:HB2	2.49	0.43
1:G:35:ASP:O	1:G:36:MET:C	2.56	0.43
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.82	0.43
1:B:111:PRO:HG2	1:B:112:TRP:CZ3	2.54	0.43
1:I:291:ASN:HD21	1:I:295:TYR:HA	1.84	0.43
1:C:403:VAL:O	1:C:428:VAL:HA	2.19	0.43
1:O:534:LEU:C	1:O:536:GLU:H	2.22	0.43
1:J:423:TYR:O	1:J:424:LYS:C	2.57	0.43
1:R:385:THR:HG21	1:R:405:ILE:HG23	2.01	0.43
1:A:203:PRO:HA	1:A:422:TYR:CG	2.54	0.43
1:J:138:VAL:HG23	1:J:170:VAL:HB	2.00	0.43
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.88	0.43
1:L:163:ALA:HB1	1:L:167:CYS:SG	2.58	0.43
1:R:569:MET:HG3	1:R:624:LEU:HG	2.00	0.43
1:C:315:GLU:HB3	1:C:318:GLN:HG3	1.99	0.43
1:G:269:MET:HG2	1:G:306:TYR:CE1	2.53	0.43
1:N:63:ASP:CB	1:N:65:LYS:N	2.72	0.43
1:D:569:MET:HA	1:D:572:SER:HB2	2.01	0.43
1:M:96:PHE:CD2	1:M:98:PRO:HD2	2.54	0.43
1:B:170:VAL:HA	1:B:171:PRO:HA	1.85	0.43
1:M:43:ASN:N	1:M:43:ASN:ND2	2.64	0.43
1:I:502:ASP:OD2	1:I:616:THR:CG2	2.65	0.43
1:M:176:VAL:CG2	1:M:236:PHE:HD2	2.31	0.43
1:E:170:VAL:HA	1:E:171:PRO:HA	1.92	0.43
1:N:327:ASP:OD1	1:N:327:ASP:C	2.58	0.43
1:R:359:TYR:CD1	1:R:359:TYR:C	2.91	0.43
1:H:67:HIS:CE1	1:H:91:THR:HG22	2.53	0.43
1:B:367:ASN:O	1:B:371:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:ASP:CG	1:O:299:ASP:H	2.22	0.43
1:H:92:ALA:HB3	1:H:118:VAL:HG22	2.00	0.43
1:B:103:ALA:O	1:B:107:THR:HB	2.19	0.43
1:Q:215:ASP:HA	1:Q:304:ALA:HA	2.00	0.43
1:N:254:ARG:O	1:N:321:GLU:HB3	2.19	0.43
1:J:274:ASP:HB2	1:J:282:PHE:CE1	2.54	0.43
1:J:547:GLU:OE2	1:J:550:ARG:CG	2.66	0.43
1:Q:566:ILE:CG2	1:Q:569:MET:CE	2.97	0.43
1:H:178:ILE:HG21	1:H:333:PHE:CZ	2.54	0.43
1:G:118:VAL:C	1:G:119:ILE:HD12	2.39	0.43
1:G:357:THR:O	1:G:360:HIS:HB3	2.19	0.43
1:C:20:GLU:HG3	1:C:20:GLU:H	1.40	0.43
1:O:71:ILE:HG21	1:O:154:THR:CG2	2.49	0.43
1:G:339:ASP:OD1	1:G:341:SER:HB2	2.18	0.43
1:H:97:LYS:N	1:H:98:PRO:CD	2.82	0.43
1:N:535:TRP:CE2	1:N:536:GLU:HG3	2.54	0.43
1:R:110:SER:C	1:R:112:TRP:H	2.23	0.43
1:N:65:LYS:HA	1:N:88:ASP:OD2	2.19	0.42
1:D:490:PRO:HB2	1:D:569:MET:CE	2.45	0.42
1:E:169:VAL:HG13	1:E:172:SER:HA	2.01	0.42
1:D:506:VAL:HG21	1:D:511:LEU:HD12	2.00	0.42
1:A:577:MET:HE2	1:A:639:PHE:CE1	2.54	0.42
1:O:275:MET:CE	1:O:283:ILE:H	2.31	0.42
1:Q:547:GLU:CD	1:Q:550:ARG:HH11	2.23	0.42
1:H:563:VAL:HG22	1:H:627:HIS:CG	2.54	0.42
1:A:550:ARG:HB2	1:A:550:ARG:NH1	2.33	0.42
1:J:51:LYS:HG3	1:J:85:GLU:OE2	2.19	0.42
1:G:159:LEU:HB2	1:G:243:GLU:HG3	2.01	0.42
1:O:379:LYS:O	1:O:381:LEU:N	2.52	0.42
1:G:291:ASN:HB3	1:G:295:TYR:HB2	2.01	0.42
1:E:621:ASP:OD1	1:E:621:ASP:N	2.52	0.42
1:H:578:TRP:CG	1:H:591:GLY:HA3	2.54	0.42
1:B:502:ASP:OD2	1:B:616:THR:HG21	2.19	0.42
1:M:627:HIS:HB2	1:M:640:GLN:HB2	2.01	0.42
1:I:77:LEU:HD11	1:I:506:VAL:HG12	2.00	0.42
1:I:162:LEU:N	1:I:162:LEU:HD13	2.34	0.42
1:J:146:LEU:HD22	1:J:176:VAL:HG12	2.01	0.42
1:P:239:ASP:OD1	1:P:277:ARG:NH2	2.52	0.42
1:L:42:ARG:HH12	1:L:140:GLU:HG2	1.75	0.42
1:O:490:PRO:HG2	1:O:543:GLY:HA3	2.01	0.42
1:M:95:VAL:HB	1:M:122:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:LYS:HE3	1:Q:337:GLY:O	2.18	0.42
1:K:534:LEU:C	1:K:536:GLU:N	2.72	0.42
1:I:416:PHE:O	1:I:420:ILE:HG13	2.18	0.42
1:I:615:ILE:HG12	1:I:618:LEU:HD22	2.01	0.42
1:F:142:PHE:HD1	1:F:146:LEU:HD12	1.80	0.42
1:M:599:GLY:O	1:M:601:PRO:HD3	2.19	0.42
1:D:180:PRO:CB	1:D:264:ILE:HD13	2.50	0.42
1:R:231:GLU:O	1:R:232:PRO:C	2.57	0.42
1:Q:553:ILE:O	1:Q:553:ILE:HG23	2.19	0.42
1:C:138:VAL:HG23	1:C:170:VAL:HB	2.01	0.42
1:K:253:VAL:HG23	1:K:253:VAL:O	2.19	0.42
1:N:308:LEU:HD12	1:N:308:LEU:HA	1.91	0.42
1:H:496:LEU:O	1:H:499:ILE:HG12	2.19	0.42
1:F:615:ILE:CG1	1:F:618:LEU:HD22	2.49	0.42
1:E:548:ILE:HD12	1:E:564:VAL:HG21	2.00	0.42
1:M:10:THR:C	1:M:12:GLU:H	2.22	0.42
1:L:470:LYS:HG2	1:L:475:ASP:HA	1.99	0.42
1:K:490:PRO:HG3	1:K:566:ILE:HG22	2.01	0.42
1:K:53:THR:HG22	1:K:168:ARG:NE	2.34	0.42
1:M:51:LYS:HD3	1:M:85:GLU:OE2	2.19	0.42
1:L:210:THR:HG21	4:L:809:HOH:O	2.18	0.42
1:O:440:SER:HA	1:O:441:PRO:HD3	1.86	0.42
1:N:550:ARG:O	1:N:560:GLN:OE1	2.37	0.42
1:H:563:VAL:HA	1:H:626:LEU:O	2.19	0.42
1:R:578:TRP:NE1	1:R:580:GLU:HG3	2.34	0.42
1:H:69:LEU:CD1	1:H:91:THR:HG23	2.49	0.42
1:A:470:LYS:NZ	1:A:554:ASP:HA	2.34	0.42
1:O:483:MET:HB3	1:O:582:GLU:CG	2.49	0.42
1:N:391:PHE:O	1:N:394:LEU:HB2	2.19	0.42
1:Q:273:ILE:O	1:Q:282:PHE:HA	2.19	0.42
1:A:503:VAL:HB	1:A:515:ASP:OD1	2.19	0.42
1:N:38:LEU:HD21	1:N:503:VAL:HA	2.00	0.42
1:H:72:GLY:O	2:H:701:SAH:N	2.53	0.42
1:O:423:TYR:HB2	1:O:425:LEU:HG	2.01	0.42
1:P:323:VAL:HB	1:P:334:SER:OG	2.19	0.42
1:G:46:PHE:CZ	1:G:140:GLU:HB3	2.54	0.42
1:L:241:GLU:HB2	1:L:277:ARG:HH21	1.85	0.42
1:J:480:GLU:HA	1:J:481:PRO:C	2.39	0.42
1:H:82:ALA:O	1:H:84:ARG:O	2.37	0.42
1:D:550:ARG:O	1:D:560:GLN:OE1	2.37	0.42
1:C:463:LEU:H	1:C:463:LEU:HD22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:84:ARG:C	1:P:86:GLY:N	2.73	0.42
1:I:145:GLU:CG	1:I:331:LEU:HD22	2.49	0.42
1:J:107:THR:HG22	1:J:108:SER:N	2.35	0.42
1:D:190:ASN:HD21	1:D:209:GLY:HA3	1.84	0.42
1:P:56:GLU:O	1:P:56:GLU:HG2	2.19	0.42
1:H:491:GLU:HG3	1:H:492:LYS:N	2.34	0.42
1:R:613:PHE:HA	1:R:614:PRO:HD2	1.93	0.42
1:O:491:GLU:HG3	1:O:492:LYS:N	2.34	0.42
1:L:178:ILE:HA	1:L:268:LEU:O	2.18	0.42
1:N:516:GLU:O	1:N:520:LYS:HG3	2.20	0.42
1:D:217:GLN:HB2	1:D:536:GLU:HB3	2.00	0.42
1:G:627:HIS:HB2	1:G:640:GLN:HB2	2.01	0.42
1:N:55:ALA:H	1:N:58:LYS:NZ	2.05	0.42
1:N:477:LEU:O	1:N:479:VAL:HG12	2.20	0.42
1:O:618:LEU:HB3	1:O:624:LEU:HD11	2.01	0.42
1:K:325:ASN:O	1:K:331:LEU:HA	2.19	0.42
1:A:577:MET:HE2	1:A:639:PHE:CZ	2.54	0.42
1:C:288:LYS:HG3	1:C:295:TYR:CZ	2.54	0.42
1:P:292:LYS:NZ	1:P:292:LYS:HA	2.34	0.42
1:G:67:HIS:CE1	1:G:91:THR:HG23	2.54	0.42
1:R:326:HIS:HA	1:R:330:SER:O	2.20	0.42
1:M:217:GLN:C	1:M:219:SER:H	2.22	0.42
1:H:123:SER:C	1:H:125:ASP:H	2.22	0.42
1:G:514:PHE:O	1:G:515:ASP:C	2.57	0.42
1:N:420:ILE:CD1	1:N:428:VAL:HG22	2.50	0.42
1:R:627:HIS:HB2	1:R:640:GLN:HB2	2.00	0.42
1:H:75:THR:HG22	1:H:514:PHE:CD1	2.55	0.42
1:L:485:VAL:HG22	1:L:487:LYS:HG3	2.01	0.42
1:Q:182:GLU:HB2	1:Q:229:LEU:HD11	2.02	0.42
1:Q:182:GLU:HG3	1:Q:263:THR:O	2.20	0.42
1:C:169:VAL:HG23	1:C:172:SER:HA	2.01	0.42
1:M:91:THR:CG2	1:M:117:THR:CG2	2.86	0.42
1:I:379:LYS:N	1:I:399:THR:CG2	2.83	0.42
1:F:399:THR:HG22	1:F:399:THR:O	2.19	0.42
1:E:434:VAL:HG13	1:E:469:LEU:CD1	2.49	0.42
1:R:497:GLN:NE2	1:R:497:GLN:H	2.11	0.42
1:M:194:ARG:O	1:M:195:LEU:C	2.58	0.42
1:F:133:ARG:HB2	1:F:164:LYS:HG3	2.02	0.42
1:G:112:TRP:O	1:G:113:SER:C	2.58	0.42
1:G:416:PHE:O	1:G:420:ILE:HG13	2.19	0.42
1:B:541:VAL:HG11	1:B:595:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:ALA:HA	1:I:162:LEU:HD22	2.00	0.42
1:L:269:MET:HG3	1:L:306:TYR:HE1	1.85	0.42
1:K:195:LEU:HB3	1:K:423:TYR:CZ	2.54	0.42
1:K:423:TYR:O	1:K:424:LYS:C	2.58	0.42
1:Q:177:TYR:CD1	1:Q:177:TYR:N	2.88	0.42
1:C:542:LYS:HA	1:C:542:LYS:HD3	1.78	0.42
1:C:272:ASP:OD1	1:C:272:ASP:C	2.58	0.42
1:E:77:LEU:O	1:E:81:MET:HG3	2.20	0.42
1:H:22:TYR:CE1	1:H:525:THR:HG22	2.54	0.42
1:F:397:ALA:O	1:F:399:THR:N	2.52	0.42
1:M:181:VAL:HG12	1:M:183:SER:HB3	2.02	0.42
1:N:96:PHE:CD2	1:N:98:PRO:HD2	2.54	0.42
1:N:27:GLU:HB3	1:N:96:PHE:CZ	2.55	0.42
1:B:182:GLU:OE2	1:B:227:ARG:NH1	2.52	0.42
1:G:96:PHE:HD2	1:G:99:MET:HG2	1.84	0.42
1:Q:323:VAL:HG23	1:Q:334:SER:O	2.20	0.42
1:I:616:THR:C	1:I:618:LEU:H	2.22	0.42
1:E:445:LEU:HD12	1:E:480:GLU:HB2	2.01	0.42
1:D:218:LEU:HD13	1:D:268:LEU:HD13	2.02	0.42
1:K:45:LYS:HE2	1:K:282:PHE:O	2.19	0.42
1:G:619:ARG:HG2	1:G:619:ARG:NH1	2.34	0.42
1:Q:395:LEU:C	1:Q:397:ALA:N	2.72	0.42
1:F:158:ALA:O	1:F:162:LEU:N	2.52	0.42
1:L:269:MET:CG	1:L:306:TYR:HE1	2.32	0.42
1:H:35:ASP:O	1:H:36:MET:C	2.57	0.42
1:C:534:LEU:HD21	1:C:611:VAL:HG11	2.02	0.42
1:F:93:LEU:HD13	1:F:123:SER:HA	2.02	0.42
1:N:316:MET:HA	1:N:317:ASN:HA	1.65	0.42
1:I:592:LEU:HD21	1:I:595:ILE:HD11	2.02	0.42
1:E:44:ASP:O	1:E:47:LEU:HB3	2.20	0.42
1:R:391:PHE:O	1:R:394:LEU:HB2	2.20	0.42
1:C:490:PRO:CB	1:C:569:MET:HE1	2.47	0.42
1:J:168:ARG:HH22	1:J:277:ARG:HB2	1.84	0.42
1:H:119:ILE:HG23	1:J:128:GLN:HG2	2.02	0.42
1:P:379:LYS:O	1:P:381:LEU:HG	2.20	0.42
1:H:169:VAL:HG11	1:H:240:PHE:O	2.20	0.42
1:F:73:THR:HG22	1:F:94:GLU:HB2	2.01	0.42
1:K:532:GLN:HG2	1:K:537:TYR:HE2	1.85	0.42
1:J:141:VAL:O	1:J:141:VAL:CG1	2.68	0.42
1:G:119:ILE:N	1:G:119:ILE:HD12	2.35	0.42
1:A:612:TYR:CZ	1:A:614:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASN:HD21	1:C:209:GLY:HA3	1.85	0.42
1:O:481:PRO:HB3	1:O:583:PHE:HD1	1.85	0.42
1:Q:55:ALA:O	1:Q:56:GLU:C	2.58	0.42
1:E:269:MET:HG2	1:E:306:TYR:HE1	1.84	0.42
1:F:229:LEU:HA	1:F:229:LEU:HD23	1.63	0.42
1:A:57:LYS:HA	1:A:57:LYS:HD2	1.82	0.42
1:F:354:SER:O	1:F:358:VAL:HG23	2.19	0.42
1:O:58:LYS:NZ	1:O:86:GLY:O	2.45	0.42
1:F:184:HIS:O	1:F:185:LEU:C	2.58	0.42
1:G:447:GLU:N	1:G:448:PRO:HA	2.35	0.42
1:E:491:GLU:HG3	1:E:540:ILE:O	2.19	0.42
1:M:451:MET:HB2	1:M:451:MET:HE2	1.93	0.42
1:C:320:PHE:C	1:C:320:PHE:CD1	2.93	0.42
1:L:631:ASP:CG	1:L:633:SER:HB2	2.40	0.42
1:M:384:ALA:O	1:M:444:VAL:HA	2.19	0.42
1:P:144:THR:O	1:P:269:MET:HE1	2.20	0.42
1:M:301:TRP:O	1:M:302:MET:HB3	2.20	0.42
1:H:51:LYS:NZ	1:H:51:LYS:HB3	2.35	0.42
1:Q:190:ASN:ND2	1:Q:209:GLY:HA3	2.29	0.42
1:I:403:VAL:HB	1:I:428:VAL:HB	2.00	0.42
1:F:91:THR:HG22	1:F:117:THR:CG2	2.50	0.42
1:A:566:ILE:O	1:A:623:SER:HA	2.20	0.42
1:J:51:LYS:HA	1:J:85:GLU:HG2	2.02	0.42
1:C:349:LEU:O	1:C:350:HIS:C	2.58	0.42
1:H:6:ILE:O	1:H:8:GLN:NE2	2.50	0.42
1:G:269:MET:HG2	1:G:306:TYR:HE1	1.84	0.42
1:N:467:GLU:OE1	1:N:557:VAL:HG13	2.20	0.42
1:I:577:MET:HA	1:I:578:TRP:CE3	2.55	0.42
1:H:574:ALA:C	1:H:575:ILE:HG13	2.40	0.42
1:H:53:THR:HG22	1:H:168:ARG:HE	1.85	0.42
1:R:3:LEU:O	1:R:15:TRP:HA	2.20	0.42
1:C:569:MET:SD	1:C:575:ILE:HD11	2.60	0.42
1:R:550:ARG:O	1:R:560:GLN:NE2	2.48	0.42
1:M:275:MET:HB2	1:M:275:MET:HE3	1.74	0.42
1:E:146:LEU:HD23	1:E:146:LEU:H	1.85	0.42
1:K:403:VAL:HB	1:K:428:VAL:HB	2.02	0.42
1:I:550:ARG:HB2	1:I:550:ARG:HH11	1.85	0.42
1:J:563:VAL:HG22	1:J:627:HIS:CD2	2.55	0.42
1:M:66:VAL:HA	1:M:135:ASP:OD2	2.20	0.42
1:J:434:VAL:HG12	1:J:469:LEU:HD13	2.01	0.42
1:B:339:ASP:OD1	1:B:341:SER:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:186:LEU:HD11	1:Q:268:LEU:HD21	2.02	0.42
1:K:310:GLU:OE2	1:K:338:LYS:HG2	2.20	0.42
1:C:412:PHE:HE2	1:C:451:MET:HG2	1.85	0.42
1:R:323:VAL:HG12	1:R:325:ASN:HD21	1.85	0.42
1:Q:618:LEU:HG	1:Q:624:LEU:HD22	2.01	0.42
1:N:227:ARG:NH2	1:N:261:SER:O	2.53	0.42
1:Q:193:PRO:HA	1:Q:362:ASN:HD21	1.84	0.42
1:M:455:ASN:HA	1:M:456:PRO:HD3	1.87	0.42
1:R:57:LYS:O	1:R:61:ASN:ND2	2.52	0.42
1:G:490:PRO:CB	1:G:569:MET:HE3	2.23	0.41
1:Q:169:VAL:HG21	1:Q:240:PHE:C	2.41	0.41
1:B:134:ALA:HB3	1:B:163:ALA:HA	2.01	0.41
1:H:84:ARG:O	1:H:85:GLU:CB	2.62	0.41
1:R:267:LEU:C	1:R:268:LEU:HD23	2.41	0.41
1:Q:191:ASP:O	1:Q:192:ILE:C	2.58	0.41
1:K:359:TYR:CZ	1:K:605:LYS:HB2	2.55	0.41
1:H:374:VAL:O	1:H:378:SER:OG	2.37	0.41
1:K:178:ILE:HA	1:K:268:LEU:O	2.20	0.41
1:C:295:TYR:C	1:C:295:TYR:CD2	2.93	0.41
1:L:39:ASP:OD2	1:L:298:ARG:HD2	2.20	0.41
1:B:59:HIS:O	1:B:61:ASN:N	2.52	0.41
1:H:97:LYS:HB2	1:H:98:PRO:HD3	2.02	0.41
1:O:179:VAL:HG11	1:O:228:GLU:HG2	2.00	0.41
1:J:447:GLU:N	1:J:448:PRO:HA	2.35	0.41
1:G:369:LYS:HB3	1:G:369:LYS:HE3	1.93	0.41
1:F:535:TRP:CG	1:F:605:LYS:HG2	2.54	0.41
1:A:505:THR:HA	1:A:509:PHE:O	2.20	0.41
1:O:216:VAL:C	1:O:302:MET:HG2	2.40	0.41
1:M:612:TYR:CE2	1:M:614:PRO:HA	2.55	0.41
1:M:416:PHE:HB2	1:M:430:ILE:HD13	2.00	0.41
1:B:522:ARG:O	1:B:526:ASP:HB2	2.19	0.41
1:G:191:ASP:OD2	1:G:194:ARG:NH1	2.42	0.41
1:M:52:THR:HG21	1:M:278:ASN:HD21	1.85	0.41
1:G:169:VAL:HG11	1:G:240:PHE:C	2.41	0.41
1:Q:231:GLU:HG2	1:Q:231:GLU:H	1.68	0.41
1:Q:269:MET:HG2	1:Q:306:TYR:CE1	2.54	0.41
1:H:387:GLY:HA2	1:H:450:TYR:CE2	2.55	0.41
1:E:550:ARG:H	1:E:560:GLN:NE2	2.13	0.41
1:B:66:VAL:CG1	1:B:67:HIS:H	2.32	0.41
1:L:280:THR:HG23	1:L:281:THR:N	2.35	0.41
1:R:54:ILE:HA	1:R:54:ILE:HD13	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:478:ARG:NH2	1:I:478:ARG:CG	2.83	0.41
1:H:178:ILE:HG21	1:H:333:PHE:CE2	2.55	0.41
1:J:478:ARG:HH21	1:J:478:ARG:CG	2.33	0.41
1:K:198:GLU:O	1:K:201:GLU:HG3	2.19	0.41
1:R:385:THR:CG2	1:R:405:ILE:HG23	2.49	0.41
1:E:96:PHE:CZ	1:E:98:PRO:HG2	2.55	0.41
1:A:570:SER:HB3	1:A:622:LYS:HG3	2.02	0.41
1:J:391:PHE:O	1:J:392:LEU:C	2.58	0.41
1:B:403:VAL:HB	1:B:428:VAL:HB	2.01	0.41
1:B:437:LEU:HD22	1:B:439:ASP:O	2.19	0.41
1:H:179:VAL:HG22	1:H:232:PRO:HA	2.02	0.41
1:O:385:THR:HB	1:O:405:ILE:HD13	2.01	0.41
1:Q:216:VAL:N	1:Q:302:MET:SD	2.93	0.41
1:I:495:ASP:C	1:I:497:GLN:NE2	2.74	0.41
1:K:136:ILE:HA	1:K:168:ARG:O	2.20	0.41
1:A:502:ASP:CG	1:A:616:THR:HG21	2.34	0.41
1:H:449:PHE:CD1	1:H:449:PHE:C	2.94	0.41
1:N:27:GLU:OE2	1:N:96:PHE:HE1	1.96	0.41
1:N:133:ARG:HH21	1:N:133:ARG:CB	2.25	0.41
1:D:291:ASN:H	1:D:292:LYS:HZ1	1.64	0.41
1:B:182:GLU:HG3	1:B:263:THR:O	2.19	0.41
1:Q:190:ASN:ND2	1:Q:190:ASN:O	2.54	0.41
1:N:548:ILE:O	1:N:549:LEU:HD13	2.21	0.41
1:I:576:PRO:HA	1:I:611:VAL:HA	2.02	0.41
1:C:228:GLU:OE2	1:C:290:LYS:NZ	2.51	0.41
1:N:275:MET:HE1	1:N:283:ILE:HG13	2.01	0.41
1:N:514:PHE:O	1:N:518:SER:HB3	2.20	0.41
1:R:84:ARG:O	1:R:85:GLU:CB	2.68	0.41
1:C:47:LEU:HD23	1:C:47:LEU:HA	1.83	0.41
1:D:357:THR:HG21	1:D:449:PHE:CZ	2.54	0.41
1:O:597:SER:HB3	1:O:598:ALA:H	1.73	0.41
1:K:6:ILE:O	1:K:8:GLN:NE2	2.53	0.41
1:M:631:ASP:O	1:M:635:GLY:N	2.50	0.41
1:Q:70:ASP:HB3	1:Q:79:SER:OG	2.20	0.41
1:H:348:GLY:O	1:H:352:MET:HG2	2.20	0.41
1:F:569:MET:HA	1:F:572:SER:HB2	2.01	0.41
1:N:54:ILE:CA	1:N:58:LYS:NZ	2.51	0.41
1:F:42:ARG:HH11	1:F:140:GLU:CG	2.30	0.41
1:E:379:LYS:HA	1:E:399:THR:HG22	1.93	0.41
1:G:83:ALA:HA	1:G:87:ALA:HB3	2.01	0.41
1:K:443:ILE:HG13	1:K:478:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:53:THR:HG22	1:O:168:ARG:HE	1.84	0.41
1:E:143:ASP:OD2	1:E:148:GLY:HA3	2.19	0.41
1:M:382:HIS:ND1	1:M:441:PRO:HA	2.35	0.41
1:A:273:ILE:HG13	1:A:275:MET:CE	2.49	0.41
1:P:39:ASP:OD2	1:P:298:ARG:CD	2.68	0.41
1:M:173:THR:CG2	1:M:174:GLY:N	2.83	0.41
1:M:173:THR:HG23	1:M:174:GLY:N	2.35	0.41
1:B:427:ASN:HA	1:C:8:GLN:NE2	2.35	0.41
1:F:264:ILE:N	1:F:312:LYS:O	2.54	0.41
1:M:235:ALA:HB1	1:M:324:CYS:HB3	2.03	0.41
1:G:562:CYS:SG	1:G:564:VAL:HG22	2.60	0.41
1:K:417:PHE:CZ	1:K:430:ILE:HB	2.55	0.41
1:J:613:PHE:HA	1:J:614:PRO:HD2	1.89	0.41
1:M:199:LYS:HA	1:M:200:ASP:HA	1.34	0.41
1:G:9:LYS:HA	1:G:9:LYS:HD2	1.72	0.41
1:H:400:ALA:O	1:H:427:ASN:ND2	2.50	0.41
1:M:153:ARG:HB2	1:M:248:PHE:CZ	2.54	0.41
1:P:107:THR:C	1:P:109:ASN:N	2.74	0.41
1:J:104:ARG:HA	1:J:118:VAL:HG21	2.02	0.41
1:E:467:GLU:OE1	1:E:556:ARG:HG3	2.21	0.41
1:P:540:ILE:HG22	1:P:542:LYS:HE3	2.03	0.41
1:O:513:PHE:O	1:O:516:GLU:HB3	2.21	0.41
1:H:535:TRP:CE3	1:H:605:LYS:HE3	2.55	0.41
1:M:68:VAL:HG22	1:M:136:ILE:CB	2.40	0.41
1:B:164:LYS:O	1:B:167:CYS:HB2	2.20	0.41
1:M:297:TRP:CE3	1:M:298:ARG:HA	2.55	0.41
1:E:84:ARG:HD3	1:O:620:ASN:HD21	1.84	0.41
1:K:218:LEU:HB2	1:K:303:GLN:NE2	2.31	0.41
1:N:216:VAL:HG13	1:N:218:LEU:HG	2.03	0.41
1:M:176:VAL:HG22	1:M:236:PHE:HB2	2.01	0.41
1:H:141:VAL:O	1:H:141:VAL:CG1	2.69	0.41
1:N:42:ARG:HH11	1:N:140:GLU:HG2	1.85	0.41
1:K:616:THR:C	1:K:618:LEU:N	2.73	0.41
1:I:129:ILE:HG22	1:I:130:GLY:N	2.36	0.41
1:P:111:PRO:HD2	1:P:112:TRP:CZ3	2.54	0.41
1:K:104:ARG:NH1	1:K:118:VAL:HG12	2.34	0.41
1:R:639:PHE:HB3	1:R:641:PHE:CE1	2.55	0.41
1:L:290:LYS:HZ2	1:L:290:LYS:HG3	1.76	0.41
1:F:180:PRO:HB2	1:F:229:LEU:HB2	2.03	0.41
1:H:109:ASN:HD22	1:H:109:ASN:N	2.18	0.41
1:B:549:LEU:HA	1:B:549:LEU:HD12	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:643:LYS:HG3	1:J:644:SER:H	1.86	0.41
1:P:259:HIS:CD2	1:P:260:SER:OG	2.54	0.41
1:N:85:GLU:N	1:N:86:GLY:HA2	2.36	0.41
1:P:316:MET:HA	1:P:317:ASN:HA	1.71	0.41
1:K:143:ASP:C	1:K:145:GLU:N	2.73	0.41
1:I:616:THR:C	1:I:618:LEU:N	2.74	0.41
1:N:36:MET:HA	1:N:300:HIS:NE2	2.35	0.41
1:C:84:ARG:HG3	1:C:112:TRP:CZ2	2.55	0.41
1:Q:110:SER:HB2	1:Q:111:PRO:HD2	2.01	0.41
1:J:618:LEU:O	1:J:620:ASN:N	2.53	0.41
1:O:632:LYS:HG3	1:O:633:SER:H	1.86	0.41
1:K:312:LYS:HD3	1:K:312:LYS:HA	1.87	0.41
1:O:390:SER:OG	1:O:447:GLU:OE1	2.33	0.41
1:O:386:VAL:HG23	1:O:446:ALA:HB2	2.02	0.41
1:L:93:LEU:CD1	1:L:123:SER:HA	2.50	0.41
1:A:16:VAL:HG11	1:C:417:PHE:CG	2.55	0.41
1:B:444:VAL:O	1:B:445:LEU:HD12	2.21	0.41
1:N:378:SER:O	1:N:379:LYS:C	2.59	0.41
1:Q:378:SER:HB2	1:Q:399:THR:CG2	2.41	0.41
1:Q:137:ILE:O	1:Q:169:VAL:HA	2.21	0.41
1:M:222:LYS:O	1:M:225:GLU:CG	2.64	0.41
1:B:314:VAL:HG22	1:B:315:GLU:N	2.30	0.41
1:G:108:SER:O	1:G:109:ASN:CB	2.67	0.41
1:J:263:THR:HA	1:J:313:LYS:HA	2.02	0.41
1:M:218:LEU:HB2	1:M:303:GLN:HE21	1.86	0.41
1:P:369:LYS:CG	1:P:370:PHE:N	2.82	0.41
1:P:45:LYS:O	1:P:275:MET:HG2	2.21	0.41
1:K:156:LYS:HG3	1:K:246:ILE:HB	2.02	0.41
1:P:297:TRP:CD2	1:P:495:ASP:HB3	2.55	0.41
1:G:239:ASP:OD1	1:G:277:ARG:NH2	2.54	0.41
1:P:27:GLU:HB3	1:P:96:PHE:CZ	2.56	0.41
1:I:553:ILE:H	1:I:553:ILE:HD12	1.86	0.41
1:K:535:TRP:O	1:K:535:TRP:CE3	2.74	0.41
1:Q:556:ARG:HB2	1:Q:556:ARG:HE	1.67	0.41
1:P:67:HIS:HE1	1:P:91:THR:HG23	1.85	0.41
1:L:180:PRO:HA	1:L:267:LEU:HD23	2.01	0.41
1:G:163:ALA:HB1	1:G:167:CYS:SG	2.61	0.41
1:J:84:ARG:HG3	1:J:112:TRP:CZ2	2.56	0.41
1:I:355:ARG:NE	3:I:702:PO4:O1	2.45	0.41
1:E:437:LEU:HD11	1:E:441:PRO:HG3	2.01	0.41
1:K:381:LEU:O	1:K:400:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:ASN:HB2	1:O:14:GLU:OE1	2.21	0.41
1:N:58:LYS:N	1:N:58:LYS:CE	2.84	0.41
1:R:471:MET:HG3	1:R:556:ARG:NH2	2.35	0.41
1:M:177:TYR:HA	1:M:233:ILE:O	2.21	0.41
1:E:57:LYS:O	1:E:66:VAL:CG2	2.58	0.41
1:O:443:ILE:HA	1:O:478:ARG:O	2.20	0.41
1:I:445:LEU:HD12	1:I:480:GLU:HB2	2.02	0.41
1:E:595:ILE:HG23	1:E:599:GLY:HA2	2.02	0.41
1:K:112:TRP:O	1:K:114:ASP:N	2.54	0.41
1:D:629:LEU:CD2	1:E:438:THR:HG21	2.48	0.41
1:P:45:LYS:HZ1	1:P:294:ASN:ND2	2.19	0.41
1:K:164:LYS:O	1:K:165:PRO:C	2.59	0.41
1:O:182:GLU:HB2	1:O:229:LEU:HD21	2.03	0.41
1:E:216:VAL:CG2	1:E:217:GLN:N	2.83	0.41
1:M:534:LEU:C	1:M:536:GLU:N	2.72	0.41
1:O:410:GLU:HB2	1:O:413:ARG:NH2	2.35	0.41
1:O:447:GLU:H	1:O:448:PRO:HA	1.85	0.41
1:I:446:ALA:HB3	1:I:462:PHE:CE1	2.56	0.41
1:L:288:LYS:HE2	1:L:288:LYS:HB3	1.63	0.41
1:N:186:LEU:HA	1:N:186:LEU:HD23	1.95	0.41
1:O:185:LEU:C	1:O:185:LEU:HD23	2.41	0.41
1:P:554:ASP:C	1:P:556:ARG:H	2.24	0.41
1:L:255:GLU:HG2	1:L:321:GLU:HG2	2.03	0.41
1:I:71:ILE:HG21	1:I:154:THR:HG23	2.02	0.41
1:G:168:ARG:NH2	1:G:276:ASP:O	2.54	0.41
1:J:493:PHE:HA	1:J:539:GLY:HA3	2.03	0.41
1:Q:485:VAL:HG12	1:Q:487:LYS:HG3	2.02	0.41
1:C:150:GLY:O	1:C:151:ALA:C	2.59	0.41
1:M:52:THR:HG21	1:M:278:ASN:ND2	2.36	0.41
1:G:169:VAL:HG11	1:G:240:PHE:O	2.21	0.41
1:A:478:ARG:NH2	1:A:478:ARG:CG	2.70	0.41
1:E:316:MET:HA	1:E:317:ASN:HA	1.86	0.41
1:P:449:PHE:HA	1:P:459:HIS:CD2	2.56	0.41
1:L:42:ARG:HH21	1:L:43:ASN:HD21	1.68	0.41
1:E:42:ARG:HE	1:E:43:ASN:ND2	2.18	0.41
1:R:550:ARG:H	1:R:560:GLN:NE2	2.18	0.41
1:J:547:GLU:OE2	1:J:550:ARG:HD2	2.21	0.41
1:H:46:PHE:CZ	1:H:140:GLU:HB2	2.56	0.41
1:I:275:MET:HE2	1:I:275:MET:CA	2.43	0.41
1:M:482:HIS:CE1	1:M:582:GLU:HB3	2.56	0.41
1:J:446:ALA:O	1:J:481:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:478:ARG:NH2	1:K:480:GLU:OE1	2.54	0.41
1:C:616:THR:C	1:C:618:LEU:H	2.24	0.41
1:K:516:GLU:CG	1:K:520:LYS:HE3	2.50	0.41
1:C:141:VAL:CG1	1:C:141:VAL:O	2.65	0.41
1:N:302:MET:HG2	1:N:303:GLN:H	1.86	0.41
1:B:38:LEU:HD13	1:B:498:ASN:HD22	1.86	0.41
1:H:268:LEU:HD12	1:H:289:TRP:HH2	1.85	0.41
1:J:119:ILE:HG22	1:J:121:GLU:HG3	2.02	0.41
1:M:487:LYS:O	1:M:577:MET:HA	2.21	0.41
1:I:190:ASN:HD21	1:I:209:GLY:HA3	1.86	0.41
1:I:243:GLU:HG2	1:I:244:GLU:N	2.34	0.41
1:G:448:PRO:HG2	1:G:448:PRO:O	2.21	0.41
1:I:455:ASN:HA	1:I:456:PRO:HD2	1.65	0.41
1:R:96:PHE:HD2	1:R:99:MET:HG2	1.85	0.41
1:E:15:TRP:NE1	1:E:520:LYS:HE2	2.36	0.41
1:M:437:LEU:HA	1:M:437:LEU:HD23	1.88	0.41
1:F:60:GLU:HG3	1:F:60:GLU:O	2.21	0.41
1:M:57:LYS:HD3	1:M:57:LYS:HA	1.96	0.41
1:E:353:LEU:HD22	1:E:357:THR:HG21	2.02	0.41
1:I:96:PHE:CZ	1:I:98:PRO:HG2	2.56	0.41
1:F:70:ASP:HA	1:F:138:VAL:O	2.20	0.41
1:J:413:ARG:NH1	1:J:432:GLU:HG3	2.36	0.41
1:H:327:ASP:C	1:H:327:ASP:OD1	2.60	0.41
1:N:427:ASN:N	1:N:427:ASN:OD1	2.53	0.41
1:D:437:LEU:HD22	1:D:437:LEU:C	2.41	0.41
1:K:623:SER:O	1:K:644:SER:OG	2.30	0.41
1:F:627:HIS:O	1:F:639:PHE:HA	2.21	0.41
1:G:185:LEU:HD23	1:G:359:TYR:HE2	1.86	0.41
1:I:326:HIS:HA	1:I:330:SER:O	2.21	0.41
1:A:186:LEU:O	1:A:187:LYS:C	2.59	0.41
1:L:105:HIS:O	1:L:109:ASN:ND2	2.46	0.41
1:L:168:ARG:CG	1:L:168:ARG:NH1	2.75	0.41
1:B:164:LYS:O	1:B:165:PRO:C	2.58	0.41
1:J:358:VAL:O	1:J:359:TYR:C	2.59	0.41
1:Q:323:VAL:HB	1:Q:334:SER:OG	2.21	0.41
1:E:383:VAL:HB	1:E:443:ILE:CG2	2.51	0.41
1:B:460:LEU:HD21	1:B:579:MET:HE2	2.02	0.41
1:G:216:VAL:CG2	1:G:217:GLN:N	2.83	0.41
1:C:420:ILE:HD11	1:C:428:VAL:HG22	2.02	0.41
1:P:445:LEU:HD12	1:P:480:GLU:HB2	2.03	0.41
1:J:455:ASN:HB3	1:J:457:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:292:LYS:HD2	1:N:293:ASN:ND2	2.37	0.41
1:D:447:GLU:N	1:D:448:PRO:HA	2.35	0.41
1:H:292:LYS:HA	1:H:293:ASN:HA	1.93	0.41
1:A:119:ILE:HG22	1:A:121:GLU:HG2	2.02	0.41
1:Q:531:GLU:HG2	1:Q:531:GLU:O	2.21	0.41
1:D:226:PHE:N	1:D:226:PHE:CD1	2.89	0.41
1:C:549:LEU:HD12	1:C:549:LEU:HA	1.68	0.41
1:K:227:ARG:NH2	1:K:261:SER:O	2.53	0.41
1:F:434:VAL:CG1	1:F:469:LEU:HD13	2.52	0.41
1:H:505:THR:HA	1:H:509:PHE:O	2.20	0.41
1:N:600:VAL:HA	1:N:601:PRO:HD3	1.85	0.41
1:Q:566:ILE:CG2	1:Q:569:MET:HE2	2.51	0.40
1:D:157:GLU:HB3	1:D:161:ARG:NH1	2.36	0.40
1:J:71:ILE:HB	1:J:139:ALA:HB2	2.02	0.40
1:F:274:ASP:OD1	1:F:277:ARG:N	2.45	0.40
1:B:37:ILE:O	1:B:37:ILE:CG2	2.68	0.40
1:B:553:ILE:O	1:B:553:ILE:HG22	2.21	0.40
1:P:447:GLU:H	1:P:448:PRO:HA	1.87	0.40
1:C:16:VAL:HG13	1:C:17:VAL:N	2.36	0.40
1:B:489:ILE:HD13	1:B:541:VAL:CG2	2.51	0.40
1:P:404:THR:HG23	1:P:429:GLU:HG3	2.03	0.40
1:K:222:LYS:HB2	1:K:225:GLU:CG	2.51	0.40
1:O:270:TRP:CE2	1:O:286:GLY:HA2	2.57	0.40
1:H:342:ARG:HH11	1:H:342:ARG:HD3	1.69	0.40
1:I:427:ASN:N	1:I:427:ASN:OD1	2.54	0.40
1:F:78:LEU:HD12	1:F:78:LEU:HA	1.83	0.40
1:B:57:LYS:O	1:B:57:LYS:HG3	2.21	0.40
1:E:178:ILE:HA	1:E:268:LEU:O	2.21	0.40
1:O:69:LEU:HD23	1:O:137:ILE:HG12	2.03	0.40
1:J:566:ILE:HG21	1:J:575:ILE:HD13	2.04	0.40
1:C:72:GLY:N	1:C:93:LEU:O	2.53	0.40
1:H:534:LEU:CD1	1:H:576:PRO:HB3	2.51	0.40
1:Q:216:VAL:CA	1:Q:302:MET:SD	3.10	0.40
1:K:277:ARG:HG2	1:K:277:ARG:O	2.21	0.40
1:L:631:ASP:C	1:L:631:ASP:OD1	2.59	0.40
1:R:460:LEU:HD21	1:R:579:MET:HE1	2.03	0.40
1:Q:460:LEU:HD22	1:Q:463:LEU:CD2	2.51	0.40
1:M:194:ARG:HB3	1:M:201:GLU:OE1	2.21	0.40
1:C:547:GLU:OE2	1:C:550:ARG:NH1	2.52	0.40
1:P:541:VAL:HG11	1:P:595:ILE:HD13	2.03	0.40
1:L:445:LEU:HD12	1:L:480:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:THR:HG22	1:J:144:THR:O	2.20	0.40
1:L:465:ASP:O	1:L:469:LEU:HD22	2.21	0.40
1:Q:287:PRO:HG2	1:Q:289:TRP:CH2	2.56	0.40
1:P:198:GLU:HB3	1:P:200:ASP:HB2	2.04	0.40
1:K:299:ASP:C	1:K:301:TRP:N	2.75	0.40
1:L:63:ASP:N	1:L:63:ASP:OD1	2.36	0.40
1:R:92:ALA:C	1:R:93:LEU:HD23	2.42	0.40
1:D:359:TYR:C	1:D:359:TYR:CD1	2.94	0.40
1:M:344:TYR:CD1	1:M:344:TYR:N	2.89	0.40
1:J:338:LYS:HA	1:J:338:LYS:HD2	1.90	0.40
1:J:40:PHE:CD1	1:J:41:ASP:N	2.90	0.40
1:G:321:GLU:O	1:G:322:ILE:HD13	2.21	0.40
1:C:59:HIS:HD2	1:C:60:GLU:HG3	1.85	0.40
1:J:297:TRP:CZ2	1:J:299:ASP:HB2	2.56	0.40
1:M:438:THR:HB	1:M:439:ASP:OD1	2.22	0.40
1:Q:474:GLY:C	1:Q:476:GLU:N	2.74	0.40
1:L:457:TRP:HA	4:L:831:HOH:O	2.20	0.40
1:F:204:LEU:HD21	1:F:419:TYR:CE1	2.56	0.40
1:D:175:ASN:ND2	1:D:237:LYS:HG2	2.37	0.40
1:A:136:ILE:HA	1:A:168:ARG:O	2.21	0.40
1:Q:179:VAL:HA	1:Q:180:PRO:HD2	1.88	0.40
1:K:549:LEU:HD12	1:K:560:GLN:HB3	2.02	0.40
1:K:175:ASN:O	1:K:271:TRP:HA	2.22	0.40
1:Q:47:LEU:O	1:Q:51:LYS:HB2	2.21	0.40
1:M:434:VAL:HG12	1:M:469:LEU:HD12	2.03	0.40
1:O:549:LEU:HA	1:O:549:LEU:HD12	1.81	0.40
1:N:140:GLU:OE1	1:N:301:TRP:CZ2	2.71	0.40
1:N:194:ARG:HB3	1:N:201:GLU:HG3	2.04	0.40
1:R:612:TYR:OH	1:R:615:ILE:CD1	2.70	0.40
1:J:261:SER:OG	1:J:315:GLU:HA	2.21	0.40
1:L:269:MET:HG2	1:L:306:TYR:CE1	2.56	0.40
1:J:392:LEU:HA	1:J:392:LEU:HD23	1.90	0.40
1:O:185:LEU:O	1:O:185:LEU:HD23	2.21	0.40
1:B:618:LEU:HD21	1:B:642:GLY:HA2	2.03	0.40
1:H:297:TRP:CE3	1:H:298:ARG:HA	2.56	0.40
1:D:631:ASP:OD1	1:D:631:ASP:C	2.59	0.40
1:Q:372:ASP:O	1:Q:376:LYS:HB2	2.21	0.40
1:P:122:ARG:O	1:P:125:ASP:HB2	2.22	0.40
1:E:578:TRP:CG	1:E:591:GLY:HA3	2.57	0.40
1:G:548:ILE:HG22	1:G:549:LEU:HD22	2.02	0.40
1:O:612:TYR:CG	1:O:613:PHE:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LYS:NZ	1:K:86:GLY:O	2.45	0.40
1:M:280:THR:CG2	1:M:281:THR:HG22	2.26	0.40
1:M:388:GLU:HB3	1:M:450:TYR:HA	2.03	0.40
1:K:497:GLN:CD	1:K:497:GLN:H	2.25	0.40
1:G:35:ASP:OD2	1:G:299:ASP:N	2.40	0.40
1:C:275:MET:CE	1:C:283:ILE:H	2.34	0.40
1:P:455:ASN:HA	1:P:456:PRO:HD3	1.89	0.40
1:O:375:ASP:HA	1:O:399:THR:OG1	2.21	0.40
1:H:460:LEU:HD21	1:H:579:MET:HE3	2.03	0.40
1:B:91:THR:HG23	1:B:119:ILE:CD1	2.52	0.40
1:N:233:ILE:HG12	1:N:256:ALA:HB2	2.04	0.40
1:I:181:VAL:HG12	1:I:266:ALA:O	2.22	0.40
1:R:111:PRO:HD2	1:R:112:TRP:CZ3	2.57	0.40
1:N:420:ILE:HA	1:N:425:LEU:HD12	2.03	0.40
1:G:448:PRO:CG	1:G:448:PRO:O	2.69	0.40
1:R:531:GLU:HA	1:R:609:GLN:O	2.21	0.40
1:H:470:LYS:HD2	1:H:555:GLY:HA3	2.04	0.40
1:N:114:ASP:N	1:N:114:ASP:OD1	2.55	0.40
1:D:181:VAL:O	1:D:265:ASP:N	2.54	0.40
1:H:315:GLU:HB3	1:H:318:GLN:HB2	2.03	0.40
1:G:310:GLU:OE1	1:G:335:ASN:OD1	2.40	0.40
1:G:227:ARG:NH2	1:G:261:SER:O	2.55	0.40
1:N:346:VAL:O	1:N:347:CYS:C	2.60	0.40
1:E:122:ARG:O	1:E:124:THR:N	2.55	0.40
1:M:388:GLU:HG2	1:M:451:MET:HG3	2.04	0.40
1:F:39:ASP:C	1:F:39:ASP:OD1	2.60	0.40
1:Q:443:ILE:CG1	1:Q:444:VAL:N	2.85	0.40
1:M:96:PHE:CE2	1:M:98:PRO:HD2	2.56	0.40
1:N:242:HIS:HB3	1:N:245:LYS:CG	2.50	0.40
1:B:168:ARG:NH2	1:B:276:ASP:O	2.55	0.40
1:M:145:GLU:O	1:M:146:LEU:HB3	2.21	0.40
1:R:278:ASN:HB2	1:R:280:THR:HG22	2.01	0.40
1:G:73:THR:HA	2:G:701:SAH:N	2.36	0.40
1:F:259:HIS:CD2	1:F:260:SER:OG	2.70	0.40
1:I:619:ARG:HG2	1:I:619:ARG:HH11	1.86	0.40
1:N:357:THR:O	1:N:361:VAL:HG23	2.22	0.40
1:O:557:VAL:CG2	1:O:632:LYS:HB2	2.49	0.40
1:D:565:ASN:ND2	1:D:644:SER:HB3	2.37	0.40
1:J:264:ILE:HD12	1:J:312:LYS:CG	2.52	0.40
1:Q:410:GLU:HG3	1:Q:413:ARG:HH22	1.87	0.40
1:N:141:VAL:O	1:N:141:VAL:CG1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:468:VAL:O	1:Q:471:MET:HB3	2.21	0.40
1:R:600:VAL:HA	1:R:601:PRO:HD2	1.82	0.40
1:M:174:GLY:HA3	1:M:273:ILE:HG22	2.03	0.40
1:E:193:PRO:HA	1:E:362:ASN:ND2	2.36	0.40
1:I:162:LEU:N	1:I:162:LEU:CD1	2.85	0.40
1:K:627:HIS:HB2	1:K:640:GLN:HB2	2.03	0.40
1:R:377:LEU:HB3	1:R:443:ILE:HD13	2.03	0.40
1:B:404:THR:HG23	1:B:429:GLU:HG3	2.03	0.40
1:O:310:GLU:OE2	1:O:338:LYS:HG2	2.22	0.40
1:D:384:ALA:O	1:D:444:VAL:HA	2.21	0.40
1:C:156:LYS:NZ	1:C:246:ILE:O	2.46	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ASP:OD1	1:C:550:ARG:NH2[3_554]	2.01	0.19
1:N:554:ASP:OD1	1:P:550:ARG:NH2[3_654]	2.09	0.11

## 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	637/655 (97%)	600 (94%)	34 (5%)	3 (0%)	34	48
1	B	634/655 (97%)	561 (88%)	62 (10%)	11 (2%)	11	14
1	C	635/655 (97%)	578 (91%)	47 (7%)	10 (2%)	12	16
1	D	633/655 (97%)	595 (94%)	34 (5%)	4 (1%)	30	43
1	E	630/655 (96%)	569 (90%)	53 (8%)	8 (1%)	15	21
1	F	634/655 (97%)	563 (89%)	62 (10%)	9 (1%)	14	19
1	G	630/655 (96%)	575 (91%)	50 (8%)	5 (1%)	24	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	635/655 (97%)	590 (93%)	39 (6%)	6 (1%)	21	30
1	I	642/655 (98%)	572 (89%)	58 (9%)	12 (2%)	10	12
1	J	642/655 (98%)	578 (90%)	54 (8%)	10 (2%)	12	16
1	K	637/655 (97%)	570 (90%)	53 (8%)	14 (2%)	8	9
1	L	642/655 (98%)	607 (94%)	34 (5%)	1 (0%)	52	69
1	M	625/655 (95%)	551 (88%)	65 (10%)	9 (1%)	14	19
1	N	634/655 (97%)	558 (88%)	67 (11%)	9 (1%)	14	19
1	O	637/655 (97%)	567 (89%)	61 (10%)	9 (1%)	14	19
1	P	630/655 (96%)	576 (91%)	48 (8%)	6 (1%)	19	28
1	Q	626/655 (96%)	526 (84%)	81 (13%)	19 (3%)	5	4
1	R	634/655 (97%)	567 (89%)	52 (8%)	15 (2%)	7	7
All	All	11417/11790 (97%)	10303 (90%)	954 (8%)	160 (1%)	14	19

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASP
1	B	59	HIS
1	B	60	GLU
1	B	278	ASN
1	F	290	LYS
1	G	87	ALA
1	I	279	GLY
1	M	35	ASP
1	M	36	MET
1	M	438	THR
1	M	616	THR
1	N	88	ASP
1	O	568	ASN
1	P	438	THR
1	Q	144	THR
1	Q	259	HIS
1	Q	336	VAL
1	R	88	ASP
1	R	219	SER
1	R	400	ALA
1	J	141	VAL
1	K	300	HIS

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Mol	Chain	Res	Type
1	A	555	GLY
1	D	277	ARG
1	D	453	ALA
1	B	77	LEU
1	B	288	LYS
1	B	555	GLY
1	C	63	ASP
1	C	289	TRP
1	C	290	LYS
1	C	617	ALA
1	F	197	GLY
1	F	278	ASN
1	F	398	LYS
1	E	87	ALA
1	E	109	ASN
1	E	123	SER
1	E	183	SER
1	H	113	SER
1	I	286	GLY
1	I	453	ALA
1	M	146	LEU
1	N	264	ILE
1	N	291	ASN
1	N	474	GLY
1	O	141	VAL
1	O	380	GLY
1	O	461	ARG
1	O	478	ARG
1	O	617	ALA
1	P	108	SER
1	P	123	SER
1	P	452	SER
1	Q	56	GLU
1	Q	219	SER
1	Q	258	ALA
1	Q	277	ARG
1	R	346	VAL
1	J	130	GLY
1	J	396	ALA
1	J	598	ALA
1	K	85	GLU
1	K	113	SER

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Mol	Chain	Res	Type
1	K	286	GLY
1	K	535	TRP
1	B	41	ASP
1	B	42	ARG
1	B	124	THR
1	C	243	GLU
1	F	148	GLY
1	G	113	SER
1	G	496	LEU
1	H	242	HIS
1	I	111	PRO
1	I	533	SER
1	M	276	ASP
1	M	289	TRP
1	Q	224	HIS
1	Q	227	ARG
1	Q	232	PRO
1	Q	340	LYS
1	R	614	PRO
1	J	597	SER
1	J	632	LYS
1	J	643	LYS
1	K	144	THR
1	K	345	CYS
1	K	453	ALA
1	K	511	LEU
1	A	291	ASN
1	B	277	ARG
1	C	33	PHE
1	C	278	ASN
1	C	316	MET
1	C	475	ASP
1	F	185	LEU
1	E	288	LYS
1	E	453	ALA
1	G	277	ARG
1	H	84	ARG
1	H	277	ARG
1	I	277	ARG
1	I	594	SER
1	I	616	THR
1	M	302	MET

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Mol	Chain	Res	Type
1	M	453	ALA
1	N	55	ALA
1	N	83	ALA
1	N	133	ARG
1	O	616	THR
1	Q	87	ALA
1	Q	243	GLU
1	Q	293	ASN
1	Q	338	LYS
1	R	52	THR
1	R	85	GLU
1	R	160	GLU
1	R	497	GLN
1	R	643	LYS
1	J	316	MET
1	K	74	GLY
1	K	617	ALA
1	B	52	THR
1	C	632	LYS
1	F	379	LYS
1	E	108	SER
1	G	57	LYS
1	H	55	ALA
1	I	556	ARG
1	P	7	ASN
1	Q	146	LEU
1	Q	632	LYS
1	R	26	GLN
1	R	243	GLU
1	J	424	LYS
1	K	290	LYS
1	K	523	THR
1	H	350	HIS
1	I	309	PRO
1	N	242	HIS
1	N	244	GLU
1	O	441	PRO
1	O	614	PRO
1	R	557	VAL
1	J	33	PHE
1	A	64	GLY
1	E	279	GLY

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Mol	Chain	Res	Type
1	R	111	PRO
1	L	111	PRO
1	D	141	VAL
1	F	615	ILE
1	P	34	GLY
1	K	197	GLY
1	F	141	VAL
1	I	553	ILE
1	R	232	PRO
1	I	232	PRO
1	Q	111	PRO
1	Q	165	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	556/569 (98%)	479 (86%)	77 (14%)	4	5
1	B	553/569 (97%)	474 (86%)	79 (14%)	4	4
1	C	554/569 (97%)	484 (87%)	70 (13%)	5	6
1	D	552/569 (97%)	488 (88%)	64 (12%)	7	9
1	E	551/569 (97%)	459 (83%)	92 (17%)	3	3
1	F	553/569 (97%)	471 (85%)	82 (15%)	4	4
1	G	552/569 (97%)	473 (86%)	79 (14%)	4	4
1	H	554/569 (97%)	481 (87%)	73 (13%)	5	6
1	I	557/569 (98%)	476 (86%)	81 (14%)	4	4
1	J	557/569 (98%)	481 (86%)	76 (14%)	5	5
1	K	556/569 (98%)	465 (84%)	91 (16%)	3	3
1	L	557/569 (98%)	483 (87%)	74 (13%)	5	6
1	M	550/569 (97%)	470 (86%)	80 (14%)	4	4
1	N	553/569 (97%)	455 (82%)	98 (18%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	556/569 (98%)	472 (85%)	84 (15%)	3	4
1	P	551/569 (97%)	469 (85%)	82 (15%)	4	4
1	Q	548/569 (96%)	465 (85%)	83 (15%)	3	4
1	R	553/569 (97%)	467 (84%)	86 (16%)	3	3
All	All	9963/10242 (97%)	8512 (85%)	1451 (15%)	4	4

All (1451) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	VAL
1	A	20	GLU
1	A	42	ARG
1	A	45	LYS
1	A	47	LEU
1	A	91	THR
1	A	107	THR
1	A	109	ASN
1	A	110	SER
1	A	117	THR
1	A	121	GLU
1	A	140	GLU
1	A	141	VAL
1	A	160	GLU
1	A	168	ARG
1	A	169	VAL
1	A	173	THR
1	A	176	VAL
1	A	185	LEU
1	A	187	LYS
1	A	191	ASP
1	A	210	THR
1	A	216	VAL
1	A	223	THR
1	A	245	LYS
1	A	253	VAL
1	A	263	THR
1	A	269	MET
1	A	281	THR
1	A	290	LYS
1	A	298	ARG

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Mol	Chain	Res	Type
1	A	305	VAL
1	A	308	LEU
1	A	314	VAL
1	A	336	VAL
1	A	338	LYS
1	A	343	SER
1	A	349	LEU
1	A	355	ARG
1	A	363	GLU
1	A	385	THR
1	A	392	LEU
1	A	398	LYS
1	A	399	THR
1	A	424	LYS
1	A	428	VAL
1	A	437	LEU
1	A	444	VAL
1	A	445	LEU
1	A	451	MET
1	A	463	LEU
1	A	469	LEU
1	A	471	MET
1	A	476	GLU
1	A	478	ARG
1	A	479	VAL
1	A	485	VAL
1	A	486	LEU
1	A	497	GLN
1	A	523	THR
1	A	532	GLN
1	A	541	VAL
1	A	546	VAL
1	A	549	LEU
1	A	554	ASP
1	A	556	ARG
1	A	558	SER
1	A	561	LYS
1	A	564	VAL
1	A	582	GLU
1	A	593	LEU
1	A	611	VAL
1	A	616	THR

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Mol	Chain	Res	Type
1	A	618	LEU
1	A	621	ASP
1	A	632	LYS
1	D	9	LYS
1	D	16	VAL
1	D	19	GLU
1	D	20	GLU
1	D	47	LEU
1	D	61	ASN
1	D	78	LEU
1	D	85	GLU
1	D	91	THR
1	D	114	ASP
1	D	117	THR
1	D	140	GLU
1	D	141	VAL
1	D	160	GLU
1	D	162	LEU
1	D	168	ARG
1	D	169	VAL
1	D	173	THR
1	D	185	LEU
1	D	187	LYS
1	D	210	THR
1	D	227	ARG
1	D	230	SER
1	D	263	THR
1	D	269	MET
1	D	281	THR
1	D	292	LYS
1	D	298	ARG
1	D	308	LEU
1	D	314	VAL
1	D	331	LEU
1	D	355	ARG
1	D	368	GLN
1	D	385	THR
1	D	392	LEU
1	D	398	LYS
1	D	399	THR
1	D	428	VAL
1	D	437	LEU

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Mol	Chain	Res	Type
1	D	438	THR
1	D	440	SER
1	D	445	LEU
1	D	451	MET
1	D	463	LEU
1	D	469	LEU
1	D	476	GLU
1	D	478	ARG
1	D	479	VAL
1	D	486	LEU
1	D	497	GLN
1	D	506	VAL
1	D	540	ILE
1	D	541	VAL
1	D	546	VAL
1	D	549	LEU
1	D	557	VAL
1	D	561	LYS
1	D	562	CYS
1	D	568	ASN
1	D	593	LEU
1	D	597	SER
1	D	611	VAL
1	D	618	LEU
1	D	622	LYS
1	B	16	VAL
1	B	19	GLU
1	B	31	SER
1	B	43	ASN
1	B	45	LYS
1	B	47	LEU
1	B	52	THR
1	B	56	GLU
1	B	62	THR
1	B	67	HIS
1	B	71	ILE
1	B	75	THR
1	B	78	LEU
1	B	84	ARG
1	B	88	ASP
1	B	101	ASP
1	B	107	THR

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Mol	Chain	Res	Type
1	B	108	SER
1	B	114	ASP
1	B	117	THR
1	B	140	GLU
1	B	162	LEU
1	B	169	VAL
1	B	173	THR
1	B	176	VAL
1	B	181	VAL
1	B	185	LEU
1	B	187	LYS
1	B	191	ASP
1	B	208	SER
1	B	210	THR
1	B	216	VAL
1	B	223	THR
1	B	230	SER
1	B	233	ILE
1	B	244	GLU
1	B	259	HIS
1	B	260	SER
1	B	263	THR
1	B	269	MET
1	B	293	ASN
1	B	298	ARG
1	B	308	LEU
1	B	331	LEU
1	B	336	VAL
1	B	351	SER
1	B	355	ARG
1	B	369	LYS
1	B	371	LYS
1	B	383	VAL
1	B	385	THR
1	B	428	VAL
1	B	436	SER
1	B	437	LEU
1	B	440	SER
1	B	451	MET
1	B	452	SER
1	B	463	LEU
1	B	469	LEU

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Mol	Chain	Res	Type
1	B	476	GLU
1	B	479	VAL
1	B	480	GLU
1	B	497	GLN
1	B	503	VAL
1	B	505	THR
1	B	507	ASN
1	B	541	VAL
1	B	546	VAL
1	B	550	ARG
1	B	557	VAL
1	B	562	CYS
1	B	570	SER
1	B	579	MET
1	B	611	VAL
1	B	614	PRO
1	B	616	THR
1	B	627	HIS
1	B	629	LEU
1	B	640	GLN
1	C	16	VAL
1	C	20	GLU
1	C	24	MET
1	C	45	LYS
1	C	47	LEU
1	C	58	LYS
1	C	62	THR
1	C	65	LYS
1	C	78	LEU
1	C	89	LYS
1	C	104	ARG
1	C	107	THR
1	C	114	ASP
1	C	117	THR
1	C	123	SER
1	C	140	GLU
1	C	162	LEU
1	C	168	ARG
1	C	173	THR
1	C	176	VAL
1	C	208	SER
1	C	210	THR

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Mol	Chain	Res	Type
1	C	230	SER
1	C	253	VAL
1	C	260	SER
1	C	269	MET
1	C	272	ASP
1	C	280	THR
1	C	288	LYS
1	C	290	LYS
1	C	293	ASN
1	C	298	ARG
1	C	305	VAL
1	C	308	LEU
1	C	311	LYS
1	C	319	THR
1	C	326	HIS
1	C	330	SER
1	C	338	LYS
1	C	355	ARG
1	C	363	GLU
1	C	383	VAL
1	C	392	LEU
1	C	428	VAL
1	C	434	VAL
1	C	437	LEU
1	C	444	VAL
1	C	445	LEU
1	C	451	MET
1	C	469	LEU
1	C	479	VAL
1	C	492	LYS
1	C	497	GLN
1	C	503	VAL
1	C	533	SER
1	C	540	ILE
1	C	549	LEU
1	C	557	VAL
1	C	561	LYS
1	C	562	CYS
1	C	568	ASN
1	C	572	SER
1	C	579	MET
1	C	593	LEU

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Mol	Chain	Res	Type
1	C	597	SER
1	C	619	ARG
1	C	621	ASP
1	C	622	LYS
1	C	629	LEU
1	C	643	LYS
1	F	1	MET
1	F	16	VAL
1	F	20	GLU
1	F	24	MET
1	F	45	LYS
1	F	47	LEU
1	F	62	THR
1	F	78	LEU
1	F	85	GLU
1	F	89	LYS
1	F	108	SER
1	F	113	SER
1	F	116	ILE
1	F	117	THR
1	F	133	ARG
1	F	140	GLU
1	F	162	LEU
1	F	169	VAL
1	F	173	THR
1	F	176	VAL
1	F	187	LYS
1	F	196	ASN
1	F	210	THR
1	F	216	VAL
1	F	243	GLU
1	F	244	GLU
1	F	253	VAL
1	F	259	HIS
1	F	263	THR
1	F	269	MET
1	F	275	MET
1	F	277	ARG
1	F	278	ASN
1	F	290	LYS
1	F	292	LYS
1	F	293	ASN

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Mol	Chain	Res	Type
1	F	298	ARG
1	F	310	GLU
1	F	316	MET
1	F	320	PHE
1	F	326	HIS
1	F	331	LEU
1	F	334	SER
1	F	335	ASN
1	F	336	VAL
1	F	341	SER
1	F	349	LEU
1	F	352	MET
1	F	355	ARG
1	F	363	GLU
1	F	383	VAL
1	F	385	THR
1	F	392	LEU
1	F	436	SER
1	F	437	LEU
1	F	444	VAL
1	F	445	LEU
1	F	451	MET
1	F	463	LEU
1	F	469	LEU
1	F	476	GLU
1	F	478	ARG
1	F	479	VAL
1	F	486	LEU
1	F	494	GLU
1	F	497	GLN
1	F	503	VAL
1	F	533	SER
1	F	540	ILE
1	F	541	VAL
1	F	546	VAL
1	F	549	LEU
1	F	550	ARG
1	F	557	VAL
1	F	564	VAL
1	F	595	ILE
1	F	602	GLU
1	F	618	LEU

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Mol	Chain	Res	Type
1	F	622	LYS
1	F	624	LEU
1	F	632	LYS
1	F	634	THR
1	E	1	MET
1	E	9	LYS
1	E	16	VAL
1	E	20	GLU
1	E	30	ARG
1	E	40	PHE
1	E	45	LYS
1	E	47	LEU
1	E	56	GLU
1	E	84	ARG
1	E	85	GLU
1	E	91	THR
1	E	93	LEU
1	E	104	ARG
1	E	107	THR
1	E	109	ASN
1	E	117	THR
1	E	121	GLU
1	E	140	GLU
1	E	144	THR
1	E	146	LEU
1	E	160	GLU
1	E	162	LEU
1	E	173	THR
1	E	176	VAL
1	E	181	VAL
1	E	185	LEU
1	E	187	LYS
1	E	199	LYS
1	E	208	SER
1	E	210	THR
1	E	216	VAL
1	E	230	SER
1	E	259	HIS
1	E	260	SER
1	E	269	MET
1	E	272	ASP
1	E	278	ASN

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Mol	Chain	Res	Type
1	E	290	LYS
1	E	298	ARG
1	E	305	VAL
1	E	308	LEU
1	E	314	VAL
1	E	317	ASN
1	E	319	THR
1	E	331	LEU
1	E	338	LYS
1	E	341	SER
1	E	343	SER
1	E	349	LEU
1	E	355	ARG
1	E	363	GLU
1	E	371	LYS
1	E	379	LYS
1	E	383	VAL
1	E	385	THR
1	E	392	LEU
1	E	399	THR
1	E	428	VAL
1	E	437	LEU
1	E	439	ASP
1	E	440	SER
1	E	444	VAL
1	E	445	LEU
1	E	451	MET
1	E	452	SER
1	E	454	MET
1	E	463	LEU
1	E	469	LEU
1	E	470	LYS
1	E	476	GLU
1	E	478	ARG
1	E	479	VAL
1	E	486	LEU
1	E	497	GLN
1	E	531	GLU
1	E	541	VAL
1	E	549	LEU
1	E	556	ARG
1	E	557	VAL

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Mol	Chain	Res	Type
1	E	561	LYS
1	E	562	CYS
1	E	571	SER
1	E	577	MET
1	E	587	ASN
1	E	593	LEU
1	E	616	THR
1	E	618	LEU
1	E	621	ASP
1	E	623	SER
1	E	632	LYS
1	E	643	LYS
1	G	1	MET
1	G	16	VAL
1	G	26	GLN
1	G	30	ARG
1	G	45	LYS
1	G	47	LEU
1	G	67	HIS
1	G	78	LEU
1	G	84	ARG
1	G	85	GLU
1	G	117	THR
1	G	122	ARG
1	G	127	SER
1	G	128	GLN
1	G	140	GLU
1	G	172	SER
1	G	176	VAL
1	G	181	VAL
1	G	185	LEU
1	G	191	ASP
1	G	199	LYS
1	G	200	ASP
1	G	206	ARG
1	G	210	THR
1	G	214	PHE
1	G	216	VAL
1	G	230	SER
1	G	243	GLU
1	G	253	VAL
1	G	260	SER

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Mol	Chain	Res	Type
1	G	261	SER
1	G	263	THR
1	G	269	MET
1	G	277	ARG
1	G	294	ASN
1	G	298	ARG
1	G	305	VAL
1	G	308	LEU
1	G	314	VAL
1	G	319	THR
1	G	336	VAL
1	G	339	ASP
1	G	341	SER
1	G	351	SER
1	G	355	ARG
1	G	371	LYS
1	G	383	VAL
1	G	385	THR
1	G	392	LEU
1	G	399	THR
1	G	424	LYS
1	G	428	VAL
1	G	433	LYS
1	G	437	LEU
1	G	444	VAL
1	G	451	MET
1	G	463	LEU
1	G	469	LEU
1	G	486	LEU
1	G	492	LYS
1	G	497	GLN
1	G	511	LEU
1	G	512	SER
1	G	533	SER
1	G	540	ILE
1	G	541	VAL
1	G	546	VAL
1	G	549	LEU
1	G	557	VAL
1	G	562	CYS
1	G	564	VAL
1	G	570	SER

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Mol	Chain	Res	Type
1	G	577	MET
1	G	587	ASN
1	G	593	LEU
1	G	597	SER
1	G	611	VAL
1	G	616	THR
1	G	629	LEU
1	H	1	MET
1	H	9	LYS
1	H	16	VAL
1	H	20	GLU
1	H	26	GLN
1	H	45	LYS
1	H	47	LEU
1	H	78	LEU
1	H	85	GLU
1	H	110	SER
1	H	114	ASP
1	H	117	THR
1	H	140	GLU
1	H	141	VAL
1	H	173	THR
1	H	181	VAL
1	H	185	LEU
1	H	210	THR
1	H	216	VAL
1	H	243	GLU
1	H	244	GLU
1	H	253	VAL
1	H	260	SER
1	H	263	THR
1	H	269	MET
1	H	281	THR
1	H	290	LYS
1	H	292	LYS
1	H	293	ASN
1	H	298	ARG
1	H	305	VAL
1	H	308	LEU
1	H	319	THR
1	H	336	VAL
1	H	338	LYS

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Mol	Chain	Res	Type
1	H	339	ASP
1	H	341	SER
1	H	351	SER
1	H	355	ARG
1	H	378	SER
1	H	385	THR
1	H	392	LEU
1	H	398	LYS
1	H	411	ARG
1	H	428	VAL
1	H	437	LEU
1	H	444	VAL
1	H	445	LEU
1	H	452	SER
1	H	463	LEU
1	H	469	LEU
1	H	475	ASP
1	H	478	ARG
1	H	479	VAL
1	H	485	VAL
1	H	486	LEU
1	H	490	PRO
1	H	497	GLN
1	H	541	VAL
1	H	546	VAL
1	H	549	LEU
1	H	556	ARG
1	H	562	CYS
1	H	564	VAL
1	H	570	SER
1	H	593	LEU
1	H	611	VAL
1	H	616	THR
1	H	618	LEU
1	H	621	ASP
1	H	632	LYS
1	H	643	LYS
1	H	644	SER
1	I	16	VAL
1	I	19	GLU
1	I	30	ARG
1	I	31	SER

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Mol	Chain	Res	Type
1	I	47	LEU
1	I	53	THR
1	I	56	GLU
1	I	63	ASP
1	I	78	LEU
1	I	85	GLU
1	I	97	LYS
1	I	104	ARG
1	I	114	ASP
1	I	115	LYS
1	I	117	THR
1	I	140	GLU
1	I	162	LEU
1	I	167	CYS
1	I	168	ARG
1	I	169	VAL
1	I	172	SER
1	I	173	THR
1	I	176	VAL
1	I	185	LEU
1	I	191	ASP
1	I	210	THR
1	I	243	GLU
1	I	261	SER
1	I	269	MET
1	I	277	ARG
1	I	278	ASN
1	I	280	THR
1	I	287	PRO
1	I	290	LYS
1	I	293	ASN
1	I	298	ARG
1	I	308	LEU
1	I	314	VAL
1	I	316	MET
1	I	325	ASN
1	I	331	LEU
1	I	336	VAL
1	I	351	SER
1	I	355	ARG
1	I	368	GLN
1	I	369	LYS

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Mol	Chain	Res	Type
1	I	383	VAL
1	I	385	THR
1	I	392	LEU
1	I	398	LYS
1	I	399	THR
1	I	424	LYS
1	I	428	VAL
1	I	437	LEU
1	I	438	THR
1	I	445	LEU
1	I	451	MET
1	I	463	LEU
1	I	469	LEU
1	I	476	GLU
1	I	478	ARG
1	I	479	VAL
1	I	486	LEU
1	I	497	GLN
1	I	541	VAL
1	I	546	VAL
1	I	549	LEU
1	I	550	ARG
1	I	554	ASP
1	I	556	ARG
1	I	557	VAL
1	I	561	LYS
1	I	564	VAL
1	I	568	ASN
1	I	572	SER
1	I	579	MET
1	I	587	ASN
1	I	593	LEU
1	I	597	SER
1	I	618	LEU
1	I	624	LEU
1	M	30	ARG
1	M	37	ILE
1	M	43	ASN
1	M	45	LYS
1	M	52	THR
1	M	56	GLU
1	M	65	LYS

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Mol	Chain	Res	Type
1	M	97	LYS
1	M	106	ILE
1	M	117	THR
1	M	119	ILE
1	M	124	THR
1	M	126	VAL
1	M	140	GLU
1	M	162	LEU
1	M	169	VAL
1	M	173	THR
1	M	175	ASN
1	M	178	ILE
1	M	185	LEU
1	M	191	ASP
1	M	194	ARG
1	M	199	LYS
1	M	200	ASP
1	M	206	ARG
1	M	210	THR
1	M	216	VAL
1	M	225	GLU
1	M	237	LYS
1	M	253	VAL
1	M	263	THR
1	M	268	LEU
1	M	269	MET
1	M	275	MET
1	M	281	THR
1	M	298	ARG
1	M	305	VAL
1	M	308	LEU
1	M	317	ASN
1	M	319	THR
1	M	326	HIS
1	M	338	LYS
1	M	351	SER
1	M	352	MET
1	M	355	ARG
1	M	369	LYS
1	M	371	LYS
1	M	383	VAL
1	M	385	THR

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Mol	Chain	Res	Type
1	M	399	THR
1	M	401	LYS
1	M	411	ARG
1	M	437	LEU
1	M	438	THR
1	M	439	ASP
1	M	444	VAL
1	M	445	LEU
1	M	451	MET
1	M	452	SER
1	M	478	ARG
1	M	479	VAL
1	M	483	MET
1	M	485	VAL
1	M	486	LEU
1	M	497	GLN
1	M	507	ASN
1	M	533	SER
1	M	540	ILE
1	M	542	LYS
1	M	547	GLU
1	M	549	LEU
1	M	554	ASP
1	M	562	CYS
1	M	568	ASN
1	M	579	MET
1	M	592	LEU
1	M	593	LEU
1	M	611	VAL
1	M	618	LEU
1	M	622	LYS
1	N	5	LYS
1	N	6	ILE
1	N	9	LYS
1	N	20	GLU
1	N	30	ARG
1	N	31	SER
1	N	47	LEU
1	N	58	LYS
1	N	62	THR
1	N	66	VAL
1	N	75	THR

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Mol	Chain	Res	Type
1	N	78	LEU
1	N	84	ARG
1	N	97	LYS
1	N	101	ASP
1	N	107	THR
1	N	108	SER
1	N	133	ARG
1	N	140	GLU
1	N	160	GLU
1	N	167	CYS
1	N	168	ARG
1	N	169	VAL
1	N	185	LEU
1	N	191	ASP
1	N	194	ARG
1	N	200	ASP
1	N	202	GLU
1	N	204	LEU
1	N	210	THR
1	N	214	PHE
1	N	237	LYS
1	N	244	GLU
1	N	245	LYS
1	N	253	VAL
1	N	259	HIS
1	N	269	MET
1	N	272	ASP
1	N	278	ASN
1	N	281	THR
1	N	294	ASN
1	N	298	ARG
1	N	305	VAL
1	N	308	LEU
1	N	313	LYS
1	N	314	VAL
1	N	317	ASN
1	N	325	ASN
1	N	331	LEU
1	N	336	VAL
1	N	341	SER
1	N	343	SER
1	N	349	LEU

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Mol	Chain	Res	Type
1	N	355	ARG
1	N	357	THR
1	N	363	GLU
1	N	371	LYS
1	N	383	VAL
1	N	385	THR
1	N	392	LEU
1	N	398	LYS
1	N	424	LYS
1	N	428	VAL
1	N	434	VAL
1	N	435	THR
1	N	436	SER
1	N	437	LEU
1	N	444	VAL
1	N	445	LEU
1	N	451	MET
1	N	454	MET
1	N	463	LEU
1	N	469	LEU
1	N	471	MET
1	N	475	ASP
1	N	476	GLU
1	N	478	ARG
1	N	479	VAL
1	N	486	LEU
1	N	492	LYS
1	N	494	GLU
1	N	497	GLN
1	N	540	ILE
1	N	541	VAL
1	N	546	VAL
1	N	549	LEU
1	N	553	ILE
1	N	557	VAL
1	N	564	VAL
1	N	593	LEU
1	N	597	SER
1	N	611	VAL
1	N	616	THR
1	N	618	LEU
1	N	621	ASP

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Mol	Chain	Res	Type
1	N	629	LEU
1	N	632	LYS
1	N	633	SER
1	O	1	MET
1	O	9	LYS
1	O	16	VAL
1	O	19	GLU
1	O	45	LYS
1	O	47	LEU
1	O	78	LEU
1	O	85	GLU
1	O	109	ASN
1	O	114	ASP
1	O	117	THR
1	O	120	SER
1	O	127	SER
1	O	128	GLN
1	O	140	GLU
1	O	141	VAL
1	O	156	LYS
1	O	162	LEU
1	O	169	VAL
1	O	176	VAL
1	O	185	LEU
1	O	187	LYS
1	O	191	ASP
1	O	206	ARG
1	O	210	THR
1	O	216	VAL
1	O	221	MET
1	O	223	THR
1	O	230	SER
1	O	233	ILE
1	O	269	MET
1	O	275	MET
1	O	281	THR
1	O	288	LYS
1	O	292	LYS
1	O	298	ARG
1	O	305	VAL
1	O	308	LEU
1	O	310	GLU

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Mol	Chain	Res	Type
1	O	313	LYS
1	O	317	ASN
1	O	319	THR
1	O	338	LYS
1	O	355	ARG
1	O	375	ASP
1	O	377	LEU
1	O	382	HIS
1	O	385	THR
1	O	399	THR
1	O	401	LYS
1	O	420	ILE
1	O	426	THR
1	O	436	SER
1	O	438	THR
1	O	445	LEU
1	O	451	MET
1	O	463	LEU
1	O	472	MET
1	O	478	ARG
1	O	486	LEU
1	O	487	LYS
1	O	497	GLN
1	O	501	SER
1	O	528	ILE
1	O	541	VAL
1	O	544	ASP
1	O	546	VAL
1	O	549	LEU
1	O	550	ARG
1	O	556	ARG
1	O	558	SER
1	O	559	SER
1	O	563	VAL
1	O	567	ASP
1	O	577	MET
1	O	579	MET
1	O	587	ASN
1	O	588	LEU
1	O	597	SER
1	O	602	GLU
1	O	621	ASP

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Mol	Chain	Res	Type
1	O	623	SER
1	O	624	LEU
1	O	643	LYS
1	P	16	VAL
1	P	45	LYS
1	P	47	LEU
1	P	58	LYS
1	P	93	LEU
1	P	104	ARG
1	P	106	ILE
1	P	108	SER
1	P	112	TRP
1	P	115	LYS
1	P	117	THR
1	P	123	SER
1	P	133	ARG
1	P	138	VAL
1	P	140	GLU
1	P	156	LYS
1	P	160	GLU
1	P	169	VAL
1	P	173	THR
1	P	176	VAL
1	P	181	VAL
1	P	187	LYS
1	P	200	ASP
1	P	210	THR
1	P	216	VAL
1	P	243	GLU
1	P	249	ASP
1	P	253	VAL
1	P	263	THR
1	P	269	MET
1	P	275	MET
1	P	290	LYS
1	P	292	LYS
1	P	298	ARG
1	P	305	VAL
1	P	308	LEU
1	P	314	VAL
1	P	316	MET
1	P	317	ASN

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Mol	Chain	Res	Type
1	P	318	GLN
1	P	319	THR
1	P	349	LEU
1	P	351	SER
1	P	352	MET
1	P	355	ARG
1	P	369	LYS
1	P	383	VAL
1	P	392	LEU
1	P	398	LYS
1	P	399	THR
1	P	433	LYS
1	P	436	SER
1	P	437	LEU
1	P	440	SER
1	P	444	VAL
1	P	445	LEU
1	P	451	MET
1	P	452	SER
1	P	463	LEU
1	P	469	LEU
1	P	470	LYS
1	P	476	GLU
1	P	478	ARG
1	P	497	GLN
1	P	505	THR
1	P	506	VAL
1	P	540	ILE
1	P	549	LEU
1	P	550	ARG
1	P	556	ARG
1	P	562	CYS
1	P	564	VAL
1	P	565	ASN
1	P	570	SER
1	P	593	LEU
1	P	611	VAL
1	P	618	LEU
1	P	621	ASP
1	P	632	LYS
1	P	640	GLN
1	P	643	LYS

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Mol	Chain	Res	Type
1	P	644	SER
1	Q	16	VAL
1	Q	30	ARG
1	Q	47	LEU
1	Q	56	GLU
1	Q	59	HIS
1	Q	78	LEU
1	Q	90	VAL
1	Q	112	TRP
1	Q	117	THR
1	Q	119	ILE
1	Q	122	ARG
1	Q	140	GLU
1	Q	153	ARG
1	Q	156	LYS
1	Q	160	GLU
1	Q	167	CYS
1	Q	168	ARG
1	Q	178	ILE
1	Q	191	ASP
1	Q	210	THR
1	Q	231	GLU
1	Q	233	ILE
1	Q	247	ILE
1	Q	259	HIS
1	Q	264	ILE
1	Q	269	MET
1	Q	273	ILE
1	Q	275	MET
1	Q	277	ARG
1	Q	290	LYS
1	Q	293	ASN
1	Q	294	ASN
1	Q	298	ARG
1	Q	305	VAL
1	Q	316	MET
1	Q	317	ASN
1	Q	318	GLN
1	Q	319	THR
1	Q	322	ILE
1	Q	325	ASN
1	Q	330	SER

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Mol	Chain	Res	Type
1	Q	334	SER
1	Q	338	LYS
1	Q	339	ASP
1	Q	340	LYS
1	Q	349	LEU
1	Q	351	SER
1	Q	355	ARG
1	Q	368	GLN
1	Q	379	LYS
1	Q	383	VAL
1	Q	392	LEU
1	Q	410	GLU
1	Q	420	ILE
1	Q	428	VAL
1	Q	437	LEU
1	Q	444	VAL
1	Q	451	MET
1	Q	469	LEU
1	Q	476	GLU
1	Q	478	ARG
1	Q	479	VAL
1	Q	480	GLU
1	Q	486	LEU
1	Q	497	GLN
1	Q	531	GLU
1	Q	533	SER
1	Q	540	ILE
1	Q	541	VAL
1	Q	546	VAL
1	Q	549	LEU
1	Q	554	ASP
1	Q	556	ARG
1	Q	563	VAL
1	Q	564	VAL
1	Q	571	SER
1	Q	588	LEU
1	Q	593	LEU
1	Q	611	VAL
1	Q	615	ILE
1	Q	618	LEU
1	Q	625	CYS
1	Q	632	LYS

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Mol	Chain	Res	Type
1	R	1	MET
1	R	5	LYS
1	R	13	ARG
1	R	19	GLU
1	R	44	ASP
1	R	45	LYS
1	R	47	LEU
1	R	51	LYS
1	R	53	THR
1	R	58	LYS
1	R	59	HIS
1	R	63	ASP
1	R	65	LYS
1	R	67	HIS
1	R	69	LEU
1	R	78	LEU
1	R	93	LEU
1	R	109	ASN
1	R	114	ASP
1	R	115	LYS
1	R	116	ILE
1	R	117	THR
1	R	124	THR
1	R	140	GLU
1	R	146	LEU
1	R	160	GLU
1	R	169	VAL
1	R	172	SER
1	R	176	VAL
1	R	178	ILE
1	R	185	LEU
1	R	191	ASP
1	R	199	LYS
1	R	206	ARG
1	R	210	THR
1	R	222	LYS
1	R	233	ILE
1	R	244	GLU
1	R	251	SER
1	R	253	VAL
1	R	269	MET
1	R	292	LYS

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Mol	Chain	Res	Type
1	R	293	ASN
1	R	294	ASN
1	R	298	ARG
1	R	305	VAL
1	R	308	LEU
1	R	315	GLU
1	R	317	ASN
1	R	331	LEU
1	R	335	ASN
1	R	349	LEU
1	R	355	ARG
1	R	364	MET
1	R	371	LYS
1	R	375	ASP
1	R	383	VAL
1	R	385	THR
1	R	392	LEU
1	R	398	LYS
1	R	401	LYS
1	R	420	ILE
1	R	433	LYS
1	R	437	LEU
1	R	451	MET
1	R	469	LEU
1	R	476	GLU
1	R	486	LEU
1	R	497	GLN
1	R	503	VAL
1	R	528	ILE
1	R	546	VAL
1	R	549	LEU
1	R	553	ILE
1	R	556	ARG
1	R	560	GLN
1	R	564	VAL
1	R	579	MET
1	R	615	ILE
1	R	616	THR
1	R	621	ASP
1	R	622	LYS
1	R	624	LEU
1	R	625	CYS

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Mol	Chain	Res	Type
1	R	638	ASN
1	R	643	LYS
1	J	5	LYS
1	J	9	LYS
1	J	16	VAL
1	J	45	LYS
1	J	47	LEU
1	J	60	GLU
1	J	62	THR
1	J	78	LEU
1	J	91	THR
1	J	107	THR
1	J	108	SER
1	J	115	LYS
1	J	132	SER
1	J	140	GLU
1	J	141	VAL
1	J	173	THR
1	J	176	VAL
1	J	181	VAL
1	J	185	LEU
1	J	191	ASP
1	J	199	LYS
1	J	210	THR
1	J	216	VAL
1	J	221	MET
1	J	222	LYS
1	J	230	SER
1	J	244	GLU
1	J	251	SER
1	J	260	SER
1	J	261	SER
1	J	263	THR
1	J	269	MET
1	J	280	THR
1	J	281	THR
1	J	288	LYS
1	J	298	ARG
1	J	308	LEU
1	J	311	LYS
1	J	319	THR
1	J	338	LYS

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Mol	Chain	Res	Type
1	J	339	ASP
1	J	351	SER
1	J	355	ARG
1	J	379	LYS
1	J	383	VAL
1	J	385	THR
1	J	398	LYS
1	J	399	THR
1	J	428	VAL
1	J	437	LEU
1	J	439	ASP
1	J	445	LEU
1	J	451	MET
1	J	461	ARG
1	J	469	LEU
1	J	476	GLU
1	J	478	ARG
1	J	485	VAL
1	J	486	LEU
1	J	492	LYS
1	J	497	GLN
1	J	509	PHE
1	J	540	ILE
1	J	541	VAL
1	J	557	VAL
1	J	558	SER
1	J	577	MET
1	J	582	GLU
1	J	593	LEU
1	J	611	VAL
1	J	616	THR
1	J	618	LEU
1	J	625	CYS
1	J	629	LEU
1	J	632	LYS
1	J	638	ASN
1	K	3	LEU
1	K	15	TRP
1	K	24	MET
1	K	31	SER
1	K	45	LYS
1	K	47	LEU

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Mol	Chain	Res	Type
1	K	60	GLU
1	K	65	LYS
1	K	66	VAL
1	K	91	THR
1	K	107	THR
1	K	112	TRP
1	K	140	GLU
1	K	141	VAL
1	K	156	LYS
1	K	160	GLU
1	K	162	LEU
1	K	169	VAL
1	K	176	VAL
1	K	181	VAL
1	K	185	LEU
1	K	191	ASP
1	K	210	THR
1	K	216	VAL
1	K	223	THR
1	K	225	GLU
1	K	227	ARG
1	K	243	GLU
1	K	244	GLU
1	K	253	VAL
1	K	257	VAL
1	K	259	HIS
1	K	263	THR
1	K	268	LEU
1	K	269	MET
1	K	273	ILE
1	K	281	THR
1	K	290	LYS
1	K	292	LYS
1	K	298	ARG
1	K	305	VAL
1	K	308	LEU
1	K	311	LYS
1	K	312	LYS
1	K	314	VAL
1	K	319	THR
1	K	321	GLU
1	K	322	ILE

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Mol	Chain	Res	Type
1	K	331	LEU
1	K	341	SER
1	K	355	ARG
1	K	363	GLU
1	K	364	MET
1	K	366	GLU
1	K	383	VAL
1	K	385	THR
1	K	392	LEU
1	K	399	THR
1	K	401	LYS
1	K	424	LYS
1	K	428	VAL
1	K	437	LEU
1	K	444	VAL
1	K	445	LEU
1	K	451	MET
1	K	469	LEU
1	K	471	MET
1	K	475	ASP
1	K	479	VAL
1	K	486	LEU
1	K	497	GLN
1	K	503	VAL
1	K	506	VAL
1	K	532	GLN
1	K	544	ASP
1	K	546	VAL
1	K	556	ARG
1	K	558	SER
1	K	562	CYS
1	K	564	VAL
1	K	567	ASP
1	K	577	MET
1	K	579	MET
1	K	589	SER
1	K	593	LEU
1	K	596	SER
1	K	597	SER
1	K	621	ASP
1	K	624	LEU
1	K	632	LYS

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Mol	Chain	Res	Type
1	K	643	LYS
1	L	47	LEU
1	L	60	GLU
1	L	62	THR
1	L	78	LEU
1	L	85	GLU
1	L	91	THR
1	L	107	THR
1	L	113	SER
1	L	114	ASP
1	L	117	THR
1	L	124	THR
1	L	128	GLN
1	L	129	ILE
1	L	140	GLU
1	L	141	VAL
1	L	162	LEU
1	L	168	ARG
1	L	169	VAL
1	L	173	THR
1	L	181	VAL
1	L	185	LEU
1	L	193	PRO
1	L	210	THR
1	L	216	VAL
1	L	221	MET
1	L	223	THR
1	L	225	GLU
1	L	228	GLU
1	L	260	SER
1	L	263	THR
1	L	269	MET
1	L	281	THR
1	L	290	LYS
1	L	298	ARG
1	L	305	VAL
1	L	308	LEU
1	L	316	MET
1	L	317	ASN
1	L	319	THR
1	L	331	LEU
1	L	349	LEU

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Mol	Chain	Res	Type
1	L	355	ARG
1	L	369	LYS
1	L	385	THR
1	L	392	LEU
1	L	399	THR
1	L	428	VAL
1	L	433	LYS
1	L	437	LEU
1	L	440	SER
1	L	444	VAL
1	L	445	LEU
1	L	451	MET
1	L	452	SER
1	L	463	LEU
1	L	469	LEU
1	L	476	GLU
1	L	479	VAL
1	L	485	VAL
1	L	486	LEU
1	L	497	GLN
1	L	503	VAL
1	L	541	VAL
1	L	549	LEU
1	L	556	ARG
1	L	557	VAL
1	L	562	CYS
1	L	564	VAL
1	L	593	LEU
1	L	611	VAL
1	L	616	THR
1	L	618	LEU
1	L	624	LEU
1	L	633	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (309) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	HIS
1	A	109	ASN
1	A	175	ASN
1	A	242	HIS

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Mol	Chain	Res	Type
1	A	259	HIS
1	A	294	ASN
1	A	303	GLN
1	A	335	ASN
1	A	362	ASN
1	A	459	HIS
1	A	482	HIS
1	A	497	GLN
1	A	498	ASN
1	A	507	ASN
1	A	587	ASN
1	D	43	ASN
1	D	67	HIS
1	D	175	ASN
1	D	190	ASN
1	D	242	HIS
1	D	259	HIS
1	D	293	ASN
1	D	303	GLN
1	D	335	ASN
1	D	362	ASN
1	D	459	HIS
1	D	482	HIS
1	D	497	GLN
1	D	507	ASN
1	D	560	GLN
1	D	565	ASN
1	B	175	ASN
1	B	190	ASN
1	B	242	HIS
1	B	259	HIS
1	B	291	ASN
1	B	294	ASN
1	B	303	GLN
1	B	335	ASN
1	B	362	ASN
1	B	455	ASN
1	B	459	HIS
1	B	482	HIS
1	B	497	GLN
1	B	498	ASN
1	B	507	ASN

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Mol	Chain	Res	Type
1	B	560	GLN
1	C	43	ASN
1	C	59	HIS
1	C	61	ASN
1	C	67	HIS
1	C	109	ASN
1	C	190	ASN
1	C	242	HIS
1	C	259	HIS
1	C	294	ASN
1	C	303	GLN
1	C	335	ASN
1	C	362	ASN
1	C	459	HIS
1	C	482	HIS
1	C	497	GLN
1	C	498	ASN
1	C	507	ASN
1	C	560	GLN
1	C	568	ASN
1	F	43	ASN
1	F	61	ASN
1	F	242	HIS
1	F	259	HIS
1	F	278	ASN
1	F	303	GLN
1	F	362	ASN
1	F	368	GLN
1	F	455	ASN
1	F	459	HIS
1	F	482	HIS
1	F	497	GLN
1	F	507	ASN
1	F	565	ASN
1	F	587	ASN
1	F	620	ASN
1	E	43	ASN
1	E	67	HIS
1	E	109	ASN
1	E	175	ASN
1	E	259	HIS
1	E	278	ASN

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Mol	Chain	Res	Type
1	E	303	GLN
1	E	317	ASN
1	E	335	ASN
1	E	362	ASN
1	E	459	HIS
1	E	482	HIS
1	E	497	GLN
1	E	507	ASN
1	E	560	GLN
1	E	587	ASN
1	E	638	ASN
1	G	43	ASN
1	G	67	HIS
1	G	109	ASN
1	G	190	ASN
1	G	259	HIS
1	G	293	ASN
1	G	294	ASN
1	G	300	HIS
1	G	303	GLN
1	G	335	ASN
1	G	362	ASN
1	G	459	HIS
1	G	482	HIS
1	G	497	GLN
1	G	560	GLN
1	G	587	ASN
1	H	26	GLN
1	H	43	ASN
1	H	67	HIS
1	H	109	ASN
1	H	175	ASN
1	H	190	ASN
1	H	224	HIS
1	H	294	ASN
1	H	303	GLN
1	H	335	ASN
1	H	362	ASN
1	H	459	HIS
1	H	482	HIS
1	H	497	GLN
1	H	507	ASN

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Mol	Chain	Res	Type
1	I	26	GLN
1	I	43	ASN
1	I	67	HIS
1	I	190	ASN
1	I	242	HIS
1	I	259	HIS
1	I	278	ASN
1	I	294	ASN
1	I	300	HIS
1	I	303	GLN
1	I	335	ASN
1	I	362	ASN
1	I	459	HIS
1	I	482	HIS
1	I	497	GLN
1	I	498	ASN
1	I	507	ASN
1	I	560	GLN
1	I	568	ASN
1	I	587	ASN
1	I	640	GLN
1	M	43	ASN
1	M	67	HIS
1	M	109	ASN
1	M	175	ASN
1	M	190	ASN
1	M	259	HIS
1	M	278	ASN
1	M	303	GLN
1	M	335	ASN
1	M	362	ASN
1	M	459	HIS
1	M	482	HIS
1	M	497	GLN
1	M	507	ASN
1	M	560	GLN
1	M	568	ASN
1	N	26	GLN
1	N	43	ASN
1	N	175	ASN
1	N	190	ASN
1	N	259	HIS

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Mol	Chain	Res	Type
1	N	291	ASN
1	N	293	ASN
1	N	294	ASN
1	N	303	GLN
1	N	335	ASN
1	N	362	ASN
1	N	459	HIS
1	N	482	HIS
1	N	497	GLN
1	N	498	ASN
1	N	507	ASN
1	N	560	GLN
1	N	565	ASN
1	O	43	ASN
1	O	67	HIS
1	O	109	ASN
1	O	175	ASN
1	O	190	ASN
1	O	303	GLN
1	O	335	ASN
1	O	362	ASN
1	O	459	HIS
1	O	497	GLN
1	O	498	ASN
1	O	507	ASN
1	O	560	GLN
1	O	565	ASN
1	O	587	ASN
1	O	620	ASN
1	O	638	ASN
1	O	640	GLN
1	P	43	ASN
1	P	67	HIS
1	P	175	ASN
1	P	190	ASN
1	P	259	HIS
1	P	294	ASN
1	P	303	GLN
1	P	317	ASN
1	P	362	ASN
1	P	459	HIS
1	P	482	HIS

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Mol	Chain	Res	Type
1	P	497	GLN
1	P	498	ASN
1	P	507	ASN
1	P	560	GLN
1	P	565	ASN
1	P	587	ASN
1	P	640	GLN
1	Q	43	ASN
1	Q	67	HIS
1	Q	175	ASN
1	Q	190	ASN
1	Q	196	ASN
1	Q	224	HIS
1	Q	242	HIS
1	Q	259	HIS
1	Q	291	ASN
1	Q	293	ASN
1	Q	300	HIS
1	Q	303	GLN
1	Q	335	ASN
1	Q	362	ASN
1	Q	455	ASN
1	Q	459	HIS
1	Q	482	HIS
1	Q	497	GLN
1	Q	498	ASN
1	Q	532	GLN
1	Q	560	GLN
1	Q	568	ASN
1	R	43	ASN
1	R	61	ASN
1	R	109	ASN
1	R	175	ASN
1	R	190	ASN
1	R	224	HIS
1	R	242	HIS
1	R	259	HIS
1	R	293	ASN
1	R	294	ASN
1	R	300	HIS
1	R	303	GLN
1	R	362	ASN

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Mol	Chain	Res	Type
1	R	459	HIS
1	R	482	HIS
1	R	497	GLN
1	R	498	ASN
1	R	560	GLN
1	R	638	ASN
1	J	43	ASN
1	J	67	HIS
1	J	175	ASN
1	J	190	ASN
1	J	242	HIS
1	J	300	HIS
1	J	303	GLN
1	J	362	ASN
1	J	459	HIS
1	J	482	HIS
1	J	497	GLN
1	J	498	ASN
1	J	627	HIS
1	K	43	ASN
1	K	67	HIS
1	K	190	ASN
1	K	259	HIS
1	K	294	ASN
1	K	303	GLN
1	K	335	ASN
1	K	362	ASN
1	K	459	HIS
1	K	482	HIS
1	K	497	GLN
1	K	498	ASN
1	K	532	GLN
1	K	560	GLN
1	K	587	ASN
1	L	26	GLN
1	L	43	ASN
1	L	61	ASN
1	L	67	HIS
1	L	175	ASN
1	L	190	ASN
1	L	242	HIS
1	L	259	HIS

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Mol	Chain	Res	Type
1	L	294	ASN
1	L	303	GLN
1	L	317	ASN
1	L	335	ASN
1	L	362	ASN
1	L	459	HIS
1	L	482	HIS
1	L	497	GLN
1	L	507	ASN
1	L	560	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 ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SAH	A	701	-	20,28,28	1.31	1 (5%)	19,40,40	2.64	9 (47%)
3	PO4	A	702	-	4,4,4	0.54	0	6,6,6	0.32	0
2	SAH	B	701	-	20,28,28	1.04	1 (5%)	19,40,40	2.32	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	B	702	-	4,4,4	0.35	0	6,6,6	0.30	0
2	SAH	C	701	-	20,28,28	1.28	2 (10%)	19,40,40	2.35	5 (26%)
3	PO4	C	702	-	4,4,4	0.35	0	6,6,6	0.29	0
2	SAH	D	701	-	20,28,28	1.27	3 (15%)	19,40,40	2.31	7 (36%)
3	PO4	D	702	-	4,4,4	0.51	0	6,6,6	0.35	0
2	SAH	E	701	-	20,28,28	1.22	3 (15%)	19,40,40	2.54	8 (42%)
3	PO4	E	702	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SAH	F	701	-	20,28,28	1.04	3 (15%)	19,40,40	2.39	7 (36%)
3	PO4	F	702	-	4,4,4	0.45	0	6,6,6	0.32	0
2	SAH	G	701	-	20,28,28	1.28	3 (15%)	19,40,40	2.59	6 (31%)
3	PO4	G	702	-	4,4,4	0.63	0	6,6,6	0.28	0
2	SAH	H	701	-	20,28,28	1.35	2 (10%)	19,40,40	3.34	6 (31%)
3	PO4	H	702	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SAH	I	701	-	20,28,28	1.15	2 (10%)	19,40,40	3.05	10 (52%)
3	PO4	I	702	-	4,4,4	0.69	0	6,6,6	0.32	0
2	SAH	J	701	-	20,28,28	1.04	2 (10%)	19,40,40	2.36	8 (42%)
3	PO4	J	702	-	4,4,4	0.62	0	6,6,6	0.28	0
2	SAH	K	701	-	20,28,28	1.21	3 (15%)	19,40,40	2.86	7 (36%)
3	PO4	K	702	-	4,4,4	0.44	0	6,6,6	0.27	0
2	SAH	L	701	-	20,28,28	1.40	2 (10%)	19,40,40	2.80	7 (36%)
3	PO4	L	702	-	4,4,4	0.61	0	6,6,6	0.29	0
2	SAH	M	701	-	20,28,28	1.64	4 (20%)	19,40,40	3.12	6 (31%)
3	PO4	M	702	-	4,4,4	0.32	0	6,6,6	0.28	0
2	SAH	N	701	-	20,28,28	1.31	3 (15%)	19,40,40	2.80	7 (36%)
3	PO4	N	702	-	4,4,4	0.43	0	6,6,6	0.29	0
2	SAH	O	701	-	20,28,28	1.19	2 (10%)	19,40,40	2.92	7 (36%)
3	PO4	O	702	-	4,4,4	0.26	0	6,6,6	0.27	0
2	SAH	P	701	-	20,28,28	1.21	1 (5%)	19,40,40	2.57	9 (47%)
3	PO4	P	702	-	4,4,4	0.51	0	6,6,6	0.30	0
2	SAH	Q	701	-	20,28,28	1.04	1 (5%)	19,40,40	2.31	3 (15%)
3	PO4	Q	702	-	4,4,4	0.50	0	6,6,6	0.27	0
2	SAH	R	701	-	20,28,28	1.10	1 (5%)	19,40,40	2.29	5 (26%)
3	PO4	R	702	-	4,4,4	0.27	0	6,6,6	0.30	0

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	SAH	A	701	-	-	0/7/31/31	0/3/3/3
3	PO4	A	702	-	-	0/0/0/0	0/0/0/0
2	SAH	B	701	-	-	0/7/31/31	0/3/3/3
3	PO4	B	702	-	-	0/0/0/0	0/0/0/0
2	SAH	C	701	-	-	0/7/31/31	0/3/3/3
3	PO4	C	702	-	-	0/0/0/0	0/0/0/0
2	SAH	D	701	-	-	0/7/31/31	0/3/3/3
3	PO4	D	702	-	-	0/0/0/0	0/0/0/0
2	SAH	E	701	-	-	0/7/31/31	0/3/3/3
3	PO4	E	702	-	-	0/0/0/0	0/0/0/0
2	SAH	F	701	-	-	0/7/31/31	0/3/3/3
3	PO4	F	702	-	-	0/0/0/0	0/0/0/0
2	SAH	G	701	-	-	0/7/31/31	0/3/3/3
3	PO4	G	702	-	-	0/0/0/0	0/0/0/0
2	SAH	H	701	-	-	0/7/31/31	0/3/3/3
3	PO4	H	702	-	-	0/0/0/0	0/0/0/0
2	SAH	I	701	-	-	0/7/31/31	0/3/3/3
3	PO4	I	702	-	-	0/0/0/0	0/0/0/0
2	SAH	J	701	-	-	0/7/31/31	0/3/3/3
3	PO4	J	702	-	-	0/0/0/0	0/0/0/0
2	SAH	K	701	-	-	0/7/31/31	0/3/3/3
3	PO4	K	702	-	-	0/0/0/0	0/0/0/0
2	SAH	L	701	-	-	0/7/31/31	0/3/3/3
3	PO4	L	702	-	-	0/0/0/0	0/0/0/0
2	SAH	M	701	-	-	0/7/31/31	0/3/3/3
3	PO4	M	702	-	-	0/0/0/0	0/0/0/0
2	SAH	N	701	-	-	0/7/31/31	0/3/3/3
3	PO4	N	702	-	-	0/0/0/0	0/0/0/0
2	SAH	O	701	-	-	0/7/31/31	0/3/3/3
3	PO4	O	702	-	-	0/0/0/0	0/0/0/0
2	SAH	P	701	-	-	0/7/31/31	0/3/3/3
3	PO4	P	702	-	-	0/0/0/0	0/0/0/0
2	SAH	Q	701	-	-	0/7/31/31	0/3/3/3
3	PO4	Q	702	-	-	0/0/0/0	0/0/0/0
2	SAH	R	701	-	-	0/7/31/31	0/3/3/3
3	PO4	R	702	-	-	0/0/0/0	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	701	SAH	C5'-SD	-2.95	1.75	1.81
2	E	701	SAH	C5'-SD	-2.60	1.76	1.81
2	D	701	SAH	C5'-SD	-2.42	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	SAH	C5'-SD	-2.12	1.77	1.81
2	I	701	SAH	O4'-C4'	-2.09	1.40	1.45
2	K	701	SAH	C5-C4	2.01	1.45	1.40
2	D	701	SAH	C2-N3	2.08	1.35	1.32
2	E	701	SAH	O4'-C1'	2.09	1.43	1.41
2	J	701	SAH	O4'-C1'	2.11	1.43	1.41
2	G	701	SAH	O4'-C1'	2.12	1.43	1.41
2	F	701	SAH	C2-N3	2.14	1.36	1.32
2	F	701	SAH	O4'-C1'	2.18	1.44	1.41
2	F	701	SAH	C5-C4	2.20	1.45	1.40
2	C	701	SAH	C5-C4	2.37	1.45	1.40
2	M	701	SAH	C2-N3	2.47	1.36	1.32
2	N	701	SAH	C4-N3	2.48	1.39	1.35
2	O	701	SAH	O4'-C1'	2.67	1.44	1.41
2	Q	701	SAH	C5-C4	2.71	1.46	1.40
2	I	701	SAH	C5-C4	2.73	1.46	1.40
2	K	701	SAH	O4'-C1'	2.75	1.44	1.41
2	O	701	SAH	C5-C4	2.77	1.46	1.40
2	N	701	SAH	C5-C4	2.83	1.46	1.40
2	J	701	SAH	C5-C4	2.85	1.46	1.40
2	B	701	SAH	C5-C4	2.87	1.47	1.40
2	H	701	SAH	C5-C4	2.93	1.47	1.40
2	E	701	SAH	C5-C4	2.98	1.47	1.40
2	M	701	SAH	C4-N3	2.99	1.40	1.35
2	D	701	SAH	C5-C4	3.06	1.47	1.40
2	R	701	SAH	C5-C4	3.18	1.47	1.40
2	A	701	SAH	C5-C4	3.30	1.47	1.40
2	L	701	SAH	C5-C4	3.31	1.48	1.40
2	M	701	SAH	O4'-C1'	3.33	1.45	1.41
2	N	701	SAH	O4'-C1'	3.35	1.45	1.41
2	G	701	SAH	C5-C4	3.38	1.48	1.40
2	H	701	SAH	C2-N3	3.45	1.38	1.32
2	P	701	SAH	C5-C4	3.55	1.48	1.40
2	M	701	SAH	C5-C4	3.66	1.48	1.40
2	C	701	SAH	O4'-C1'	4.03	1.46	1.41
2	L	701	SAH	O4'-C1'	4.13	1.46	1.41

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	701	SAH	N3-C2-N1	-9.20	121.85	128.89
2	I	701	SAH	N3-C2-N1	-9.14	121.90	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	701	SAH	N3-C2-N1	-8.53	122.36	128.89
2	O	701	SAH	N3-C2-N1	-8.46	122.42	128.89
2	M	701	SAH	N3-C2-N1	-8.16	122.64	128.89
2	Q	701	SAH	N3-C2-N1	-8.03	122.75	128.89
2	H	701	SAH	N3-C2-N1	-7.86	122.88	128.89
2	R	701	SAH	N3-C2-N1	-7.85	122.88	128.89
2	F	701	SAH	N3-C2-N1	-7.81	122.92	128.89
2	E	701	SAH	N3-C2-N1	-7.70	123.00	128.89
2	P	701	SAH	N3-C2-N1	-7.62	123.06	128.89
2	K	701	SAH	N3-C2-N1	-7.41	123.22	128.89
2	G	701	SAH	N3-C2-N1	-7.39	123.24	128.89
2	B	701	SAH	N3-C2-N1	-7.23	123.36	128.89
2	C	701	SAH	N3-C2-N1	-7.18	123.39	128.89
2	A	701	SAH	N3-C2-N1	-6.95	123.57	128.89
2	H	701	SAH	O4'-C1'-N9	-6.23	95.05	108.10
2	J	701	SAH	N3-C2-N1	-6.22	124.13	128.89
2	K	701	SAH	O4'-C1'-N9	-5.92	95.70	108.10
2	D	701	SAH	N3-C2-N1	-5.69	124.54	128.89
2	I	701	SAH	C1'-N9-C4	-5.11	119.23	126.94
2	G	701	SAH	C2'-C1'-N9	-4.93	106.77	114.29
2	J	701	SAH	O4'-C1'-N9	-4.57	98.54	108.10
2	A	701	SAH	O4'-C1'-N9	-4.54	98.60	108.10
2	O	701	SAH	O4'-C1'-N9	-4.14	99.43	108.10
2	P	701	SAH	C1'-N9-C4	-4.11	120.75	126.94
2	K	701	SAH	C1'-N9-C4	-3.99	120.92	126.94
2	D	701	SAH	O4'-C1'-N9	-3.83	100.09	108.10
2	I	701	SAH	CB-CG-SD	-3.60	106.64	113.57
2	G	701	SAH	C4-C5-N7	-3.59	106.18	109.48
2	D	701	SAH	CB-CG-SD	-3.55	106.72	113.57
2	L	701	SAH	C4-C5-N7	-3.47	106.28	109.48
2	I	701	SAH	C4-C5-N7	-3.42	106.34	109.48
2	G	701	SAH	CB-CG-SD	-3.42	106.99	113.57
2	L	701	SAH	O4'-C1'-N9	-3.40	100.98	108.10
2	L	701	SAH	C1'-N9-C4	-3.27	122.01	126.94
2	E	701	SAH	O4'-C1'-N9	-3.23	101.34	108.10
2	J	701	SAH	C1'-N9-C4	-3.22	122.08	126.94
2	L	701	SAH	CB-CG-SD	-3.19	107.42	113.57
2	F	701	SAH	C1'-N9-C4	-3.17	122.16	126.94
2	M	701	SAH	O4'-C1'-N9	-3.15	101.50	108.10
2	E	701	SAH	C4'-C5'-SD	-3.09	103.99	113.53
2	N	701	SAH	C1'-N9-C4	-3.08	122.29	126.94
2	H	701	SAH	CB-CG-SD	-3.07	107.66	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	SAH	C1'-N9-C4	-3.03	122.36	126.94
2	A	701	SAH	O3'-C3'-C4'	-3.03	101.96	111.05
2	E	701	SAH	C1'-N9-C4	-2.93	122.52	126.94
2	C	701	SAH	C4-C5-N7	-2.93	106.79	109.48
2	H	701	SAH	C4-C5-N7	-2.82	106.88	109.48
2	P	701	SAH	C4-C5-N7	-2.80	106.90	109.48
2	B	701	SAH	C4-C5-N7	-2.78	106.92	109.48
2	R	701	SAH	CB-CG-SD	-2.77	108.24	113.57
2	D	701	SAH	O3'-C3'-C4'	-2.76	102.76	111.05
2	E	701	SAH	C4-C5-N7	-2.74	106.96	109.48
2	O	701	SAH	CB-CG-SD	-2.66	108.44	113.57
2	C	701	SAH	O4'-C1'-N9	-2.66	102.54	108.10
2	Q	701	SAH	CB-CG-SD	-2.61	108.53	113.57
2	N	701	SAH	CB-CG-SD	-2.61	108.54	113.57
2	O	701	SAH	C1'-N9-C4	-2.61	123.01	126.94
2	B	701	SAH	O3'-C3'-C2'	-2.60	103.38	111.83
2	I	701	SAH	O3'-C3'-C4'	-2.58	103.33	111.05
2	J	701	SAH	C4-C5-N7	-2.56	107.12	109.48
2	J	701	SAH	O3'-C3'-C4'	-2.53	103.47	111.05
2	L	701	SAH	O3'-C3'-C4'	-2.48	103.60	111.05
2	E	701	SAH	O3'-C3'-C4'	-2.47	103.65	111.05
2	D	701	SAH	C4-C5-N7	-2.42	107.25	109.48
2	A	701	SAH	CB-CG-SD	-2.42	108.91	113.57
2	F	701	SAH	C4-C5-N7	-2.39	107.28	109.48
2	R	701	SAH	C4-C5-N7	-2.39	107.28	109.48
2	C	701	SAH	O3'-C3'-C4'	-2.38	103.91	111.05
2	I	701	SAH	C5'-SD-CG	-2.32	95.46	102.41
2	B	701	SAH	O4'-C1'-N9	-2.28	103.32	108.10
2	P	701	SAH	O3'-C3'-C4'	-2.16	104.57	111.05
2	R	701	SAH	C4'-C5'-SD	-2.12	106.98	113.53
2	I	701	SAH	C4'-C5'-SD	-2.09	107.09	113.53
2	K	701	SAH	C4-C5-N7	-2.04	107.60	109.48
2	P	701	SAH	CB-CG-SD	-2.04	109.65	113.57
2	A	701	SAH	C4-C5-N7	-2.02	107.62	109.48
2	J	701	SAH	CB-CG-SD	-2.00	109.71	113.57
2	A	701	SAH	C2-N1-C6	2.06	122.44	118.77
2	E	701	SAH	C2'-C1'-N9	2.08	117.47	114.29
2	P	701	SAH	C2-N1-C6	2.09	122.51	118.77
2	K	701	SAH	C2'-C3'-C4'	2.10	106.93	102.61
2	F	701	SAH	C4'-O4'-C1'	2.13	112.06	109.72
2	F	701	SAH	CB-CA-N	2.14	116.60	110.52
2	K	701	SAH	C2-N1-C6	2.14	122.60	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	701	SAH	N6-C6-N1	2.16	123.84	119.20
2	E	701	SAH	C4'-O4'-C1'	2.16	112.10	109.72
2	J	701	SAH	C2'-C1'-N9	2.18	117.62	114.29
2	A	701	SAH	C2'-C3'-C4'	2.22	107.18	102.61
2	M	701	SAH	C2-N1-C6	2.28	122.85	118.77
2	J	701	SAH	C2'-C3'-C4'	2.29	107.31	102.61
2	P	701	SAH	C2'-C3'-C4'	2.30	107.34	102.61
2	G	701	SAH	C2-N1-C6	2.32	122.92	118.77
2	Q	701	SAH	C4'-O4'-C1'	2.33	112.28	109.72
2	R	701	SAH	C2-N1-C6	2.34	122.95	118.77
2	I	701	SAH	C2-N1-C6	2.35	122.97	118.77
2	N	701	SAH	CB-CA-N	2.35	117.21	110.52
2	D	701	SAH	C4'-O4'-C1'	2.40	112.35	109.72
2	B	701	SAH	C2'-C3'-C4'	2.42	107.58	102.61
2	G	701	SAH	O4'-C1'-N9	2.43	113.19	108.10
2	F	701	SAH	C2'-C3'-C4'	2.44	107.63	102.61
2	N	701	SAH	C2-N1-C6	2.55	123.33	118.77
2	B	701	SAH	C4'-O4'-C1'	2.60	112.57	109.72
2	F	701	SAH	C2'-C1'-N9	2.65	118.34	114.29
2	P	701	SAH	C2'-C1'-N9	2.77	118.53	114.29
2	O	701	SAH	C2'-C3'-C4'	2.79	108.36	102.61
2	I	701	SAH	C2'-C3'-C4'	2.81	108.38	102.61
2	O	701	SAH	C4'-O4'-C1'	2.86	112.86	109.72
2	I	701	SAH	C4'-O4'-C1'	2.86	112.87	109.72
2	P	701	SAH	C4'-O4'-C1'	3.00	113.02	109.72
2	D	701	SAH	C2'-C1'-N9	3.03	118.92	114.29
2	M	701	SAH	N6-C6-N1	3.30	126.30	119.20
2	L	701	SAH	C2'-C1'-N9	3.68	119.91	114.29
2	N	701	SAH	C2'-C1'-N9	3.95	120.32	114.29
2	A	701	SAH	C2'-C1'-N9	4.01	120.42	114.29
2	C	701	SAH	C2'-C1'-N9	4.42	121.05	114.29
2	M	701	SAH	C4'-O4'-C1'	4.78	114.97	109.72
2	H	701	SAH	C4'-O4'-C1'	4.80	115.00	109.72
2	K	701	SAH	C2'-C1'-N9	5.06	122.03	114.29
2	O	701	SAH	C2'-C1'-N9	5.31	122.41	114.29
2	H	701	SAH	C2'-C1'-N9	7.17	125.25	114.29
2	M	701	SAH	C2'-C1'-N9	7.58	125.88	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	SAH	2	0
2	C	701	SAH	1	0
2	E	701	SAH	3	0
2	F	701	SAH	2	0
2	G	701	SAH	2	0
2	H	701	SAH	1	0
2	I	701	SAH	1	0
3	I	702	PO4	1	0
2	K	701	SAH	3	0
2	M	701	SAH	2	0
2	N	701	SAH	1	0
2	P	701	SAH	3	0
2	Q	701	SAH	1	0
3	Q	702	PO4	1	0
2	R	701	SAH	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	641/655 (97%)	0.04	1 (0%) 95 95	16, 33, 57, 83	0
1	B	638/655 (97%)	0.15	7 (1%) 82 82	24, 43, 74, 103	0
1	C	639/655 (97%)	0.09	1 (0%) 95 95	26, 44, 68, 100	0
1	D	637/655 (97%)	0.04	1 (0%) 95 95	19, 34, 56, 101	0
1	E	636/655 (97%)	0.21	10 (1%) 74 74	21, 41, 80, 124	0
1	F	638/655 (97%)	0.21	13 (2%) 68 68	27, 48, 75, 120	0
1	G	636/655 (97%)	0.15	12 (1%) 70 69	23, 43, 81, 129	0
1	H	639/655 (97%)	0.03	1 (0%) 95 95	18, 38, 60, 91	0
1	I	644/655 (98%)	0.05	5 (0%) 87 87	28, 44, 68, 94	0
1	J	644/655 (98%)	0.15	6 (0%) 85 85	29, 47, 69, 92	0
1	K	641/655 (97%)	0.19	8 (1%) 81 81	26, 52, 77, 99	0
1	L	644/655 (98%)	0.02	2 (0%) 94 94	19, 33, 55, 78	0
1	M	633/655 (96%)	0.46	41 (6%) 22 22	38, 61, 84, 110	0
1	N	638/655 (97%)	0.21	7 (1%) 82 82	36, 55, 75, 93	0
1	O	641/655 (97%)	0.49	43 (6%) 21 21	39, 64, 96, 127	0
1	P	636/655 (97%)	0.25	32 (5%) 32 33	30, 51, 82, 105	0
1	Q	632/655 (96%)	0.52	52 (8%) 14 14	37, 62, 99, 124	0
1	R	638/655 (97%)	0.66	65 (10%) 9 8	44, 69, 99, 131	0
All	All	11495/11790 (97%)	0.22	307 (2%) 58 57	16, 48, 82, 131	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	586	ILE	9.0
1	E	64	GLY	6.8
1	E	119	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	O	644	SER	5.6
1	Q	116	ILE	5.5
1	Q	86	GLY	5.2
1	O	553	ILE	5.2
1	R	54	ILE	5.1
1	R	68	VAL	5.0
1	G	114	ASP	4.8
1	R	598	ALA	4.7
1	Q	155	PHE	4.7
1	M	107	THR	4.7
1	R	599	GLY	4.6
1	R	264	ILE	4.5
1	O	377	LEU	4.5
1	Q	329	PHE	4.4
1	F	317	ASN	4.4
1	O	595	ILE	4.3
1	R	199	LYS	4.3
1	R	60	GLU	4.3
1	O	583	PHE	4.3
1	M	106	ILE	4.3
1	R	40	PHE	4.3
1	R	257	VAL	4.2
1	Q	340	LYS	4.1
1	P	136	ILE	4.1
1	O	557	VAL	4.0
1	R	66	VAL	4.0
1	Q	257	VAL	4.0
1	F	315	GLU	3.9
1	G	164	LYS	3.9
1	Q	311	LYS	3.9
1	Q	437	LEU	3.9
1	D	62	THR	3.8
1	R	222	LYS	3.8
1	Q	236	PHE	3.8
1	R	320	PHE	3.7
1	R	162	LEU	3.7
1	N	54	ILE	3.7
1	E	118	VAL	3.7
1	M	66	VAL	3.7
1	R	50	LEU	3.6
1	M	48	ALA	3.6
1	O	633	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	316	MET	3.6
1	F	262	GLY	3.6
1	O	564	VAL	3.6
1	R	593	LEU	3.6
1	E	66	VAL	3.6
1	P	55	ALA	3.6
1	Q	262	GLY	3.6
1	P	137	ILE	3.5
1	G	121	GLU	3.5
1	R	200	ASP	3.5
1	O	577	MET	3.5
1	O	620	ASN	3.5
1	M	566	ILE	3.5
1	O	426	THR	3.5
1	K	62	THR	3.5
1	O	566	ILE	3.4
1	P	86	GLY	3.4
1	R	428	VAL	3.4
1	Q	336	VAL	3.4
1	M	514	PHE	3.3
1	Q	119	ILE	3.3
1	M	555	GLY	3.3
1	P	114	ASP	3.3
1	M	301	TRP	3.3
1	F	336	VAL	3.3
1	O	517	ILE	3.3
1	Q	59	HIS	3.3
1	P	66	VAL	3.3
1	R	602	GLU	3.2
1	R	477	LEU	3.2
1	R	55	ALA	3.2
1	M	82	ALA	3.2
1	I	129	ILE	3.2
1	O	199	LYS	3.2
1	P	555	GLY	3.2
1	Q	90	VAL	3.2
1	R	155	PHE	3.1
1	R	444	VAL	3.1
1	I	622	LYS	3.1
1	P	93	LEU	3.1
1	R	88	ASP	3.1
1	K	489	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	118	VAL	3.1
1	R	58	LYS	3.1
1	P	74	GLY	3.1
1	N	320	PHE	3.1
1	J	292	LYS	3.1
1	Q	317	ASN	3.1
1	Q	308	LEU	3.0
1	M	643	LYS	3.0
1	I	66	VAL	3.0
1	M	238	PHE	3.0
1	P	155	PHE	3.0
1	E	93	LEU	3.0
1	P	454	MET	3.0
1	P	132	SER	2.9
1	E	114	ASP	2.9
1	Q	337	GLY	2.9
1	F	189	PHE	2.9
1	M	50	LEU	2.9
1	M	180	PRO	2.9
1	R	159	LEU	2.9
1	P	67	HIS	2.9
1	O	585	GLY	2.9
1	Q	93	LEU	2.9
1	Q	555	GLY	2.9
1	K	454	MET	2.9
1	M	314	VAL	2.9
1	Q	253	VAL	2.9
1	Q	247	ILE	2.9
1	O	320	PHE	2.9
1	Q	137	ILE	2.9
1	O	483	MET	2.9
1	O	379	LYS	2.9
1	L	131	GLY	2.8
1	M	52	THR	2.8
1	O	629	LEU	2.8
1	J	454	MET	2.8
1	O	584	GLY	2.8
1	R	234	VAL	2.8
1	P	546	VAL	2.8
1	F	556	ARG	2.8
1	F	320	PHE	2.8
1	M	206	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	347	CYS	2.8
1	R	425	LEU	2.8
1	R	179	VAL	2.7
1	R	246	ILE	2.7
1	R	471	MET	2.7
1	E	111	PRO	2.7
1	E	570	SER	2.7
1	P	240	PHE	2.7
1	Q	240	PHE	2.7
1	F	316	MET	2.7
1	R	296	ALA	2.7
1	P	314	VAL	2.7
1	G	162	LEU	2.6
1	M	318	GLN	2.6
1	Q	158	ALA	2.6
1	Q	556	ARG	2.6
1	Q	162	LEU	2.6
1	R	478	ARG	2.6
1	N	134	ALA	2.6
1	L	454	MET	2.6
1	O	489	ILE	2.6
1	O	540	ILE	2.6
1	Q	314	VAL	2.6
1	K	114	ASP	2.6
1	M	46	PHE	2.6
1	O	565	ASN	2.6
1	P	68	VAL	2.6
1	M	210	THR	2.6
1	J	227	ARG	2.6
1	Q	112	TRP	2.6
1	O	486	LEU	2.6
1	R	308	LEU	2.6
1	M	119	ILE	2.6
1	M	247	ILE	2.6
1	Q	319	THR	2.5
1	O	551	PHE	2.5
1	Q	238	PHE	2.5
1	P	509	PHE	2.5
1	R	167	CYS	2.5
1	M	61	ASN	2.5
1	M	103	ALA	2.5
1	R	622	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	Q	627	HIS	2.5
1	R	85	GLU	2.5
1	M	624	LEU	2.5
1	Q	292	LYS	2.5
1	Q	111	PRO	2.5
1	G	116	ILE	2.5
1	B	133	ARG	2.5
1	O	545	ALA	2.4
1	R	505	THR	2.4
1	Q	255	GLU	2.4
1	Q	277	ARG	2.4
1	J	315	GLU	2.4
1	B	292	LYS	2.4
1	R	142	PHE	2.4
1	R	59	HIS	2.4
1	O	192	ILE	2.4
1	O	428	VAL	2.4
1	B	83	ALA	2.4
1	M	65	LYS	2.4
1	R	511	LEU	2.4
1	F	370	PHE	2.4
1	F	613	PHE	2.4
1	N	294	ASN	2.4
1	Q	161	ARG	2.4
1	N	268	LEU	2.4
1	G	68	VAL	2.4
1	Q	163	ALA	2.4
1	R	62	THR	2.4
1	I	292	LYS	2.4
1	R	643	LYS	2.4
1	M	320	PHE	2.4
1	B	113	SER	2.3
1	Q	57	LYS	2.3
1	P	63	ASP	2.3
1	O	561	LYS	2.3
1	R	164	LYS	2.3
1	J	586	ILE	2.3
1	Q	85	GLU	2.3
1	E	132	SER	2.3
1	F	54	ILE	2.3
1	N	319	THR	2.3
1	F	282	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	369	LYS	2.3
1	O	443	ILE	2.3
1	O	399	THR	2.3
1	Q	133	ARG	2.3
1	M	623	SER	2.3
1	B	199	LYS	2.3
1	O	349	LEU	2.3
1	P	133	ARG	2.3
1	O	403	VAL	2.3
1	R	443	ILE	2.3
1	R	504	GLY	2.3
1	O	477	LEU	2.3
1	G	54	ILE	2.2
1	R	600	VAL	2.2
1	R	571	SER	2.2
1	Q	199	LYS	2.2
1	O	200	ASP	2.2
1	G	161	ARG	2.2
1	P	69	LEU	2.2
1	Q	267	LEU	2.2
1	G	59	HIS	2.2
1	R	283	ILE	2.2
1	P	620	ASN	2.2
1	P	58	LYS	2.2
1	O	567	ASP	2.2
1	R	456	PRO	2.2
1	R	592	LEU	2.2
1	G	158	ALA	2.2
1	M	55	ALA	2.2
1	B	169	VAL	2.2
1	R	621	ASP	2.2
1	M	471	MET	2.2
1	R	38	LEU	2.2
1	P	628	ALA	2.2
1	M	116	ILE	2.2
1	M	17	VAL	2.2
1	R	314	VAL	2.2
1	P	644	SER	2.2
1	R	345	CYS	2.2
1	R	206	ARG	2.1
1	M	142	PHE	2.1
1	P	51	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	586	ILE	2.1
1	K	611	VAL	2.1
1	Q	232	PRO	2.1
1	M	313	LYS	2.1
1	O	622	LYS	2.1
1	M	199	LYS	2.1
1	R	340	LYS	2.1
1	H	556	ARG	2.1
1	P	619	ARG	2.1
1	R	454	MET	2.1
1	K	624	LEU	2.1
1	M	168	ARG	2.1
1	Q	66	VAL	2.1
1	Q	234	VAL	2.1
1	M	155	PHE	2.1
1	P	40	PHE	2.1
1	R	80	LEU	2.1
1	K	545	ALA	2.1
1	M	224	HIS	2.1
1	N	322	ILE	2.1
1	F	280	THR	2.1
1	M	64	GLY	2.1
1	Q	241	GLU	2.1
1	R	359	TYR	2.1
1	P	134	ALA	2.1
1	E	63	ASP	2.1
1	B	132	SER	2.1
1	M	261	SER	2.1
1	O	541	VAL	2.1
1	M	40	PHE	2.0
1	R	282	PHE	2.0
1	G	78	LEU	2.0
1	O	469	LEU	2.0
1	Q	89	LYS	2.0
1	Q	341	SER	2.0
1	O	315	GLU	2.0
1	C	137	ILE	2.0
1	A	555	GLY	2.0
1	R	194	ARG	2.0
1	P	89	LYS	2.0
1	R	513	PHE	2.0
1	K	55	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	347	CYS	2.0
1	G	132	SER	2.0
1	O	619	ARG	2.0
1	P	117	THR	2.0
1	Q	117	THR	2.0
1	Q	179	VAL	2.0
1	R	138	VAL	2.0
1	J	544	ASP	2.0
1	Q	50	LEU	2.0
1	Q	334	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAH	D	701	26/26	0.95	0.15	0.82	32,37,45,46	0
2	SAH	R	701	26/26	0.91	0.17	0.28	47,56,92,99	0
2	SAH	M	701	26/26	0.89	0.16	-0.03	36,61,74,79	0
3	PO4	M	702	5/5	0.91	0.13	-0.05	70,71,74,78	0
2	SAH	C	701	26/26	0.95	0.14	-0.12	36,48,57,59	0
2	SAH	F	701	26/26	0.95	0.14	-0.22	35,46,61,64	0
2	SAH	A	701	26/26	0.96	0.13	-0.33	27,33,38,38	0
2	SAH	G	701	26/26	0.93	0.14	-0.42	46,63,72,72	0
2	SAH	Q	701	26/26	0.92	0.14	-0.43	48,64,75,76	0
2	SAH	E	701	26/26	0.95	0.13	-0.51	43,53,63,65	0
2	SAH	B	701	26/26	0.96	0.12	-0.61	36,43,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAH	N	701	26/26	0.90	0.12	-0.63	40,53,58,58	0
2	SAH	K	701	26/26	0.94	0.13	-0.73	37,41,47,51	0
2	SAH	H	701	26/26	0.96	0.12	-0.79	24,29,33,34	0
2	SAH	I	701	26/26	0.96	0.12	-0.89	35,38,45,47	0
2	SAH	P	701	26/26	0.93	0.11	-0.98	43,53,63,65	0
2	SAH	J	701	26/26	0.96	0.11	-1.10	34,38,44,46	0
2	SAH	L	701	26/26	0.97	0.12	-1.22	27,33,36,39	0
3	PO4	E	702	5/5	0.98	0.11	-1.26	36,40,43,47	0
2	SAH	O	701	26/26	0.95	0.10	-1.42	37,41,47,52	0
3	PO4	O	702	5/5	0.97	0.07	-1.69	57,58,70,72	0
3	PO4	K	702	5/5	0.98	0.09	-2.54	43,45,46,51	0
3	PO4	A	702	5/5	0.99	0.12	-	31,32,37,39	0
3	PO4	N	702	5/5	0.97	0.09	-	52,57,62,66	0
3	PO4	G	702	5/5	0.99	0.11	-	42,42,49,50	0
3	PO4	H	702	5/5	0.98	0.09	-	28,34,36,37	0
3	PO4	L	702	5/5	0.99	0.12	-	32,32,35,37	0
3	PO4	D	702	5/5	0.99	0.12	-	31,35,36,37	0
3	PO4	J	702	5/5	0.98	0.11	-	45,46,49,51	0
3	PO4	Q	702	5/5	0.96	0.12	-	59,63,72,72	0
3	PO4	F	702	5/5	0.98	0.08	-	38,42,49,56	0
3	PO4	P	702	5/5	0.98	0.12	-	43,43,45,47	0
3	PO4	R	702	5/5	0.96	0.09	-	52,55,59,61	0
3	PO4	I	702	5/5	0.97	0.14	-	36,37,44,49	0
3	PO4	C	702	5/5	0.98	0.09	-	37,41,44,44	0
3	PO4	B	702	5/5	0.98	0.13	-	36,39,45,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.