



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2017 – 05:33 PM EST

PDB ID : 3FI0  
Title : Crystal Structure Analysis of B. stearothermophilus Tryptophanyl-tRNA Synthetase Complexed with Tryptophan, AMP, and Inorganic Phosphate  
Authors : Laowanapiban, P.; Kapustina, M.; Vonrhein, C.; Delarue, M.; Koehl, P.; Carter Jr., C.W.  
Deposited on : unknown  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

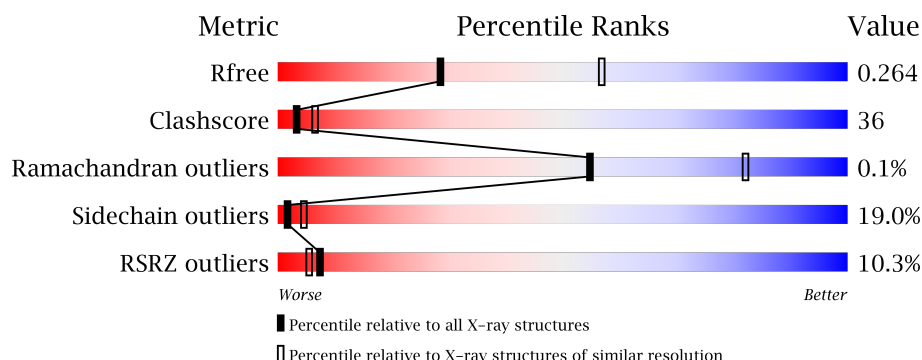
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	326	<div> <div>4%</div> <div> <div></div> <div>48%</div> <div>36%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	326	<div> <div>8%</div> <div> <div></div> <div>38%</div> <div>41%</div> <div>11%</div> <div>10%</div> </div> </div>
1	C	326	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>39%</div> <div>7%</div> <div>9%</div> </div> </div>
1	D	326	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>34%</div> <div>6%</div> <div>8%</div> </div> </div>
1	E	326	<div> <div>13%</div> <div> <div></div> <div>36%</div> <div>44%</div> <div>10%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	326	
1	G	326	
1	H	326	
1	I	326	
1	J	326	
1	K	326	
1	L	326	
1	M	326	
1	N	326	
1	O	326	
1	P	326	
1	Q	326	
1	R	326	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRP	B	1001	-	-	-	X
2	TRP	H	1001	-	-	-	X
2	TRP	O	1001	-	-	-	X
3	PO4	E	1002	-	-	X	-
3	PO4	F	1002	-	-	X	-
3	PO4	H	1002	-	-	X	-
3	PO4	M	1002	-	-	X	-
3	PO4	N	1002	-	-	X	-
3	PO4	O	1002	-	-	X	-
3	PO4	P	1002	-	-	X	-
4	AMP	A	1003	-	-	X	X
4	AMP	B	1003	-	-	X	X
4	AMP	C	1003	-	-	-	X
4	AMP	D	1003	-	-	-	X
4	AMP	E	1003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	F	1003	-	-	-	X
4	AMP	G	1003	-	-	X	X
4	AMP	H	1003	-	-	-	X
4	AMP	I	1003	-	-	X	X
4	AMP	J	1003	-	-	-	X
4	AMP	K	1003	-	-	-	X
4	AMP	L	1003	-	-	-	X
4	AMP	M	1003	-	-	-	X
4	AMP	N	1003	-	-	-	X
4	AMP	O	1003	-	-	X	X
4	AMP	P	1003	-	-	X	X
4	AMP	Q	1003	-	-	X	X
4	AMP	R	1003	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43727 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	B	295	Total	C	N	O	S	Se	0	0	0
			2370	1505	408	444	3	10			
1	C	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	D	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	E	293	Total	C	N	O	S	Se	0	0	0
			2342	1484	405	440	3	10			
1	F	296	Total	C	N	O	S	Se	0	0	0
			2368	1502	410	443	3	10			
1	G	302	Total	C	N	O	S	Se	0	0	0
			2416	1534	416	453	3	10			
1	H	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	I	298	Total	C	N	O	S	Se	0	0	0
			2377	1507	409	448	3	10			
1	J	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	K	296	Total	C	N	O	S	Se	0	0	0
			2367	1504	408	442	3	10			
1	L	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	M	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	N	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	O	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	P	295	Total	C	N	O	S	Se	0	0	0
			2361	1499	407	442	3	10			

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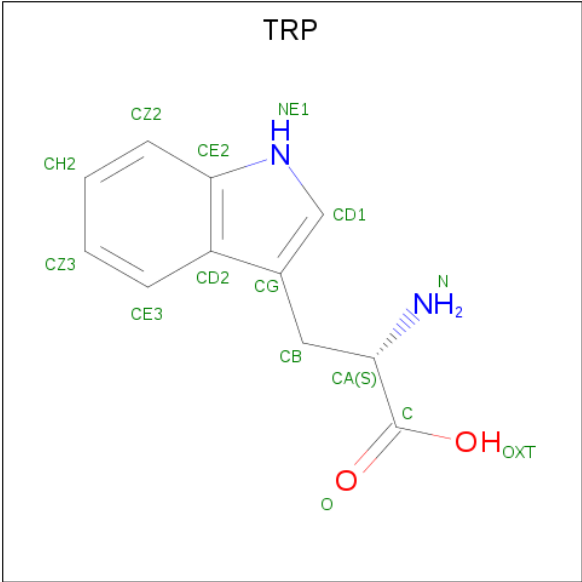
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	R	290	Total	C	N	O	S	Se	0	0	0
			2322	1473	399	437	3	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	LYS	CONFLICT	UNP P00953
D	64	LEU	LYS	CONFLICT	UNP P00953
B	64	LEU	LYS	CONFLICT	UNP P00953
C	64	LEU	LYS	CONFLICT	UNP P00953
E	64	LEU	LYS	CONFLICT	UNP P00953
F	64	LEU	LYS	CONFLICT	UNP P00953
G	64	LEU	LYS	CONFLICT	UNP P00953
H	64	LEU	LYS	CONFLICT	UNP P00953
I	64	LEU	LYS	CONFLICT	UNP P00953
J	64	LEU	LYS	CONFLICT	UNP P00953
K	64	LEU	LYS	CONFLICT	UNP P00953
L	64	LEU	LYS	CONFLICT	UNP P00953
M	64	LEU	LYS	CONFLICT	UNP P00953
N	64	LEU	LYS	CONFLICT	UNP P00953
O	64	LEU	LYS	CONFLICT	UNP P00953
P	64	LEU	LYS	CONFLICT	UNP P00953
Q	64	LEU	LYS	CONFLICT	UNP P00953
R	64	LEU	LYS	CONFLICT	UNP P00953

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



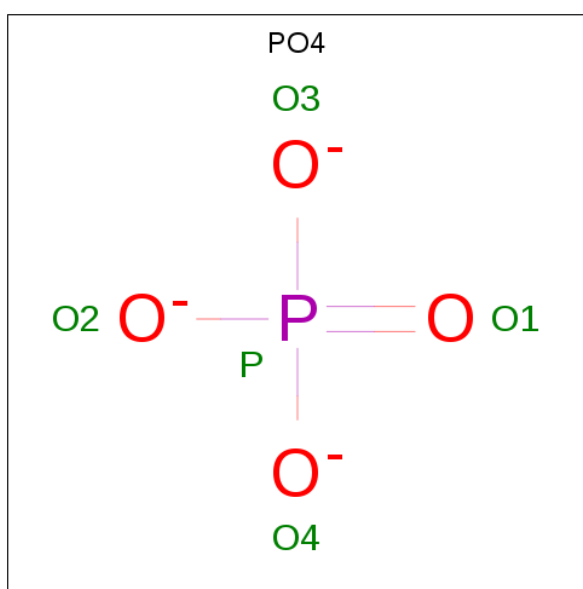
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		
2	I	1	Total	C	N	O	0	0
			15	11	2	2		
2	J	1	Total	C	N	O	0	0
			15	11	2	2		
2	K	1	Total	C	N	O	0	0
			15	11	2	2		
2	L	1	Total	C	N	O	0	0
			15	11	2	2		
2	M	1	Total	C	N	O	0	0
			15	11	2	2		
2	N	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			15	11	2	2		
2	P	1	Total	C	N	O	0	0
			15	11	2	2		
2	Q	1	Total	C	N	O	0	0
			15	11	2	2		
2	R	1	Total	C	N	O	0	0
			15	11	2	2		

- 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	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

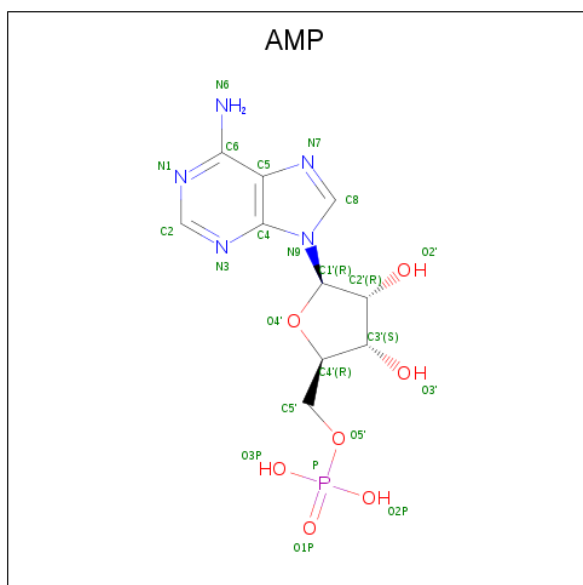
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).

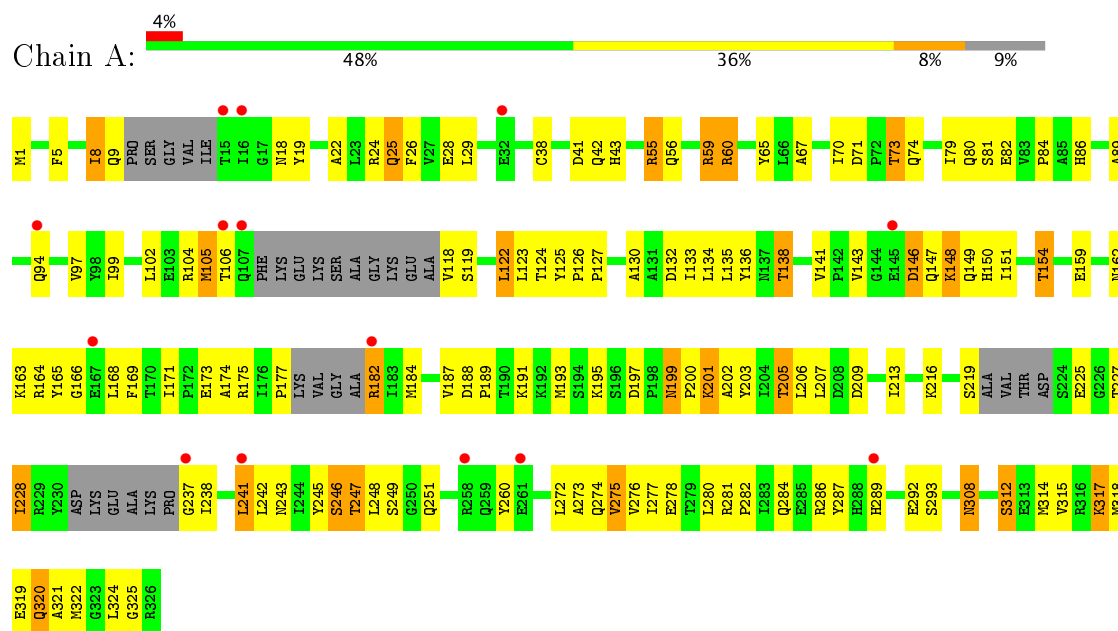


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	I	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	J	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	K	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	L	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	M	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	N	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	O	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	P	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	R	1	Total 23	C 10	N 5	O 7	P 1	0	0

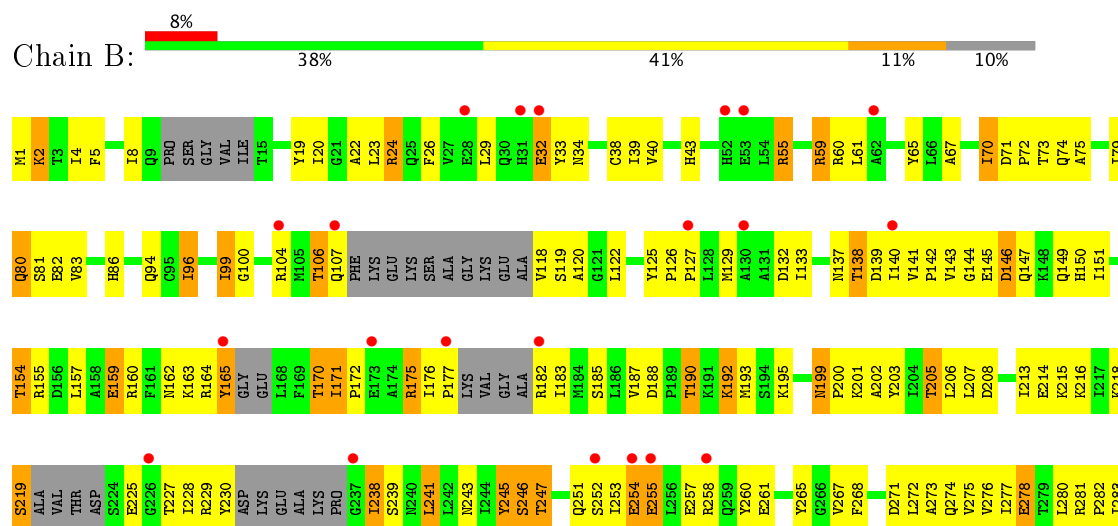
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Tryptophanyl-tRNA synthetase

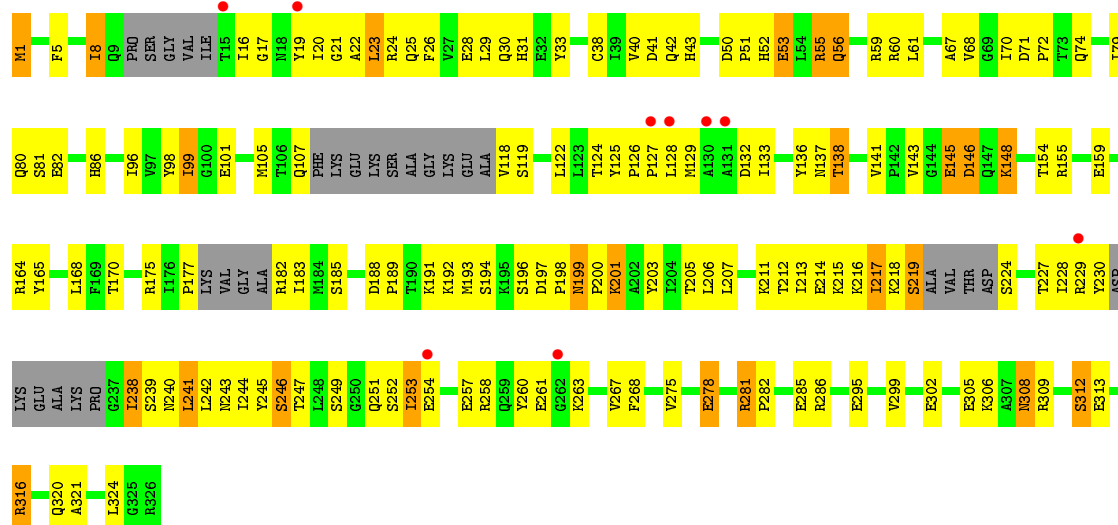
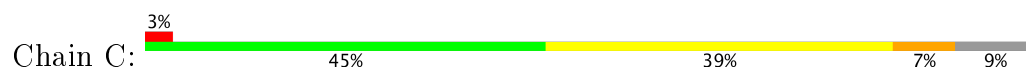


#### • Molecule 1: Tryptophanyl-tRNA synthetase

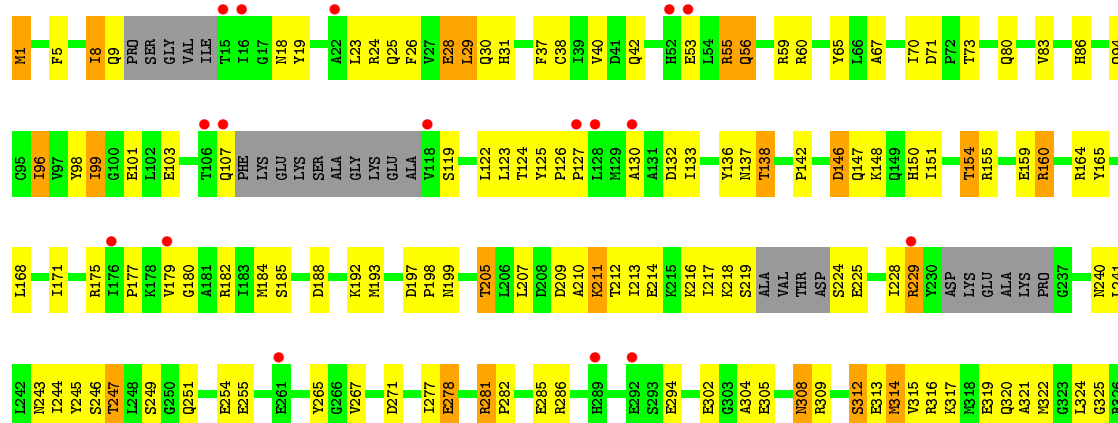




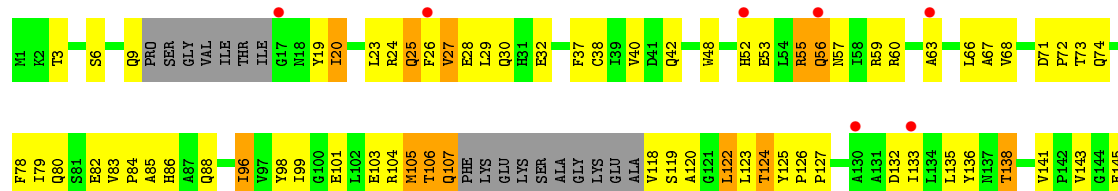
• Molecule 1: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase

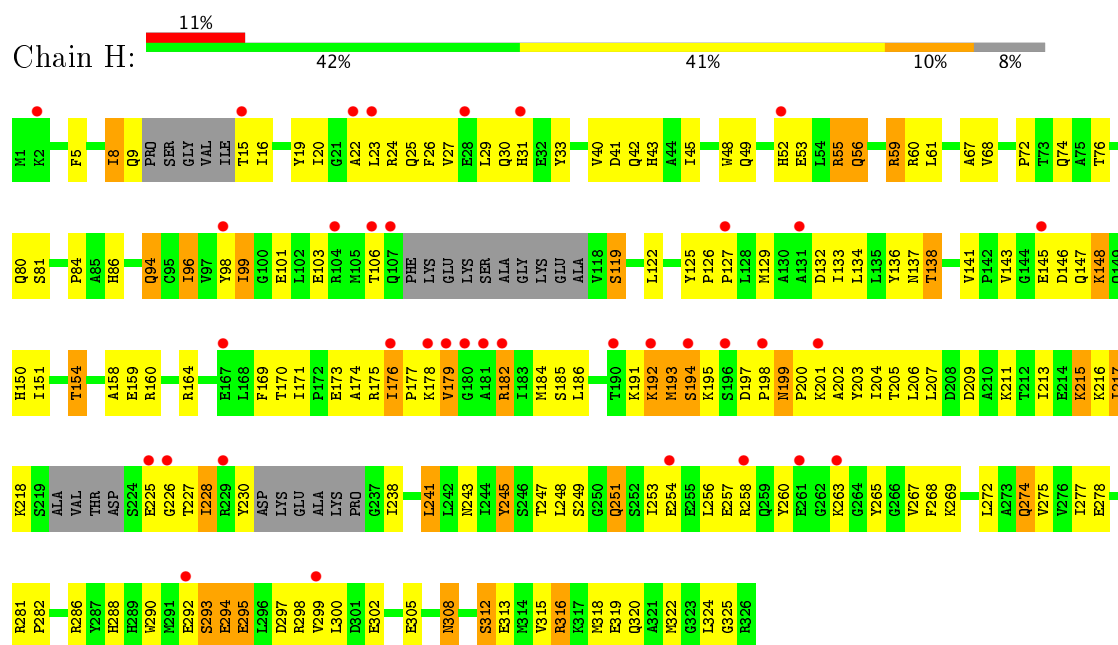


• Molecule 1: Tryptophanyl-tRNA synthetase



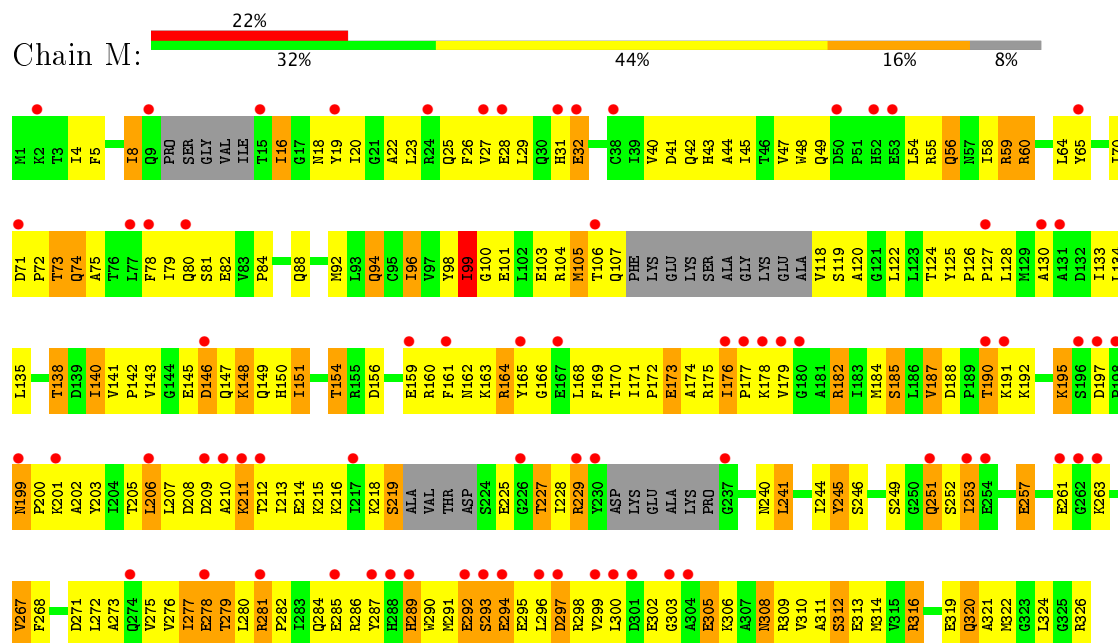


- Molecule 1: Tryptophanyl-tRNA synthetase

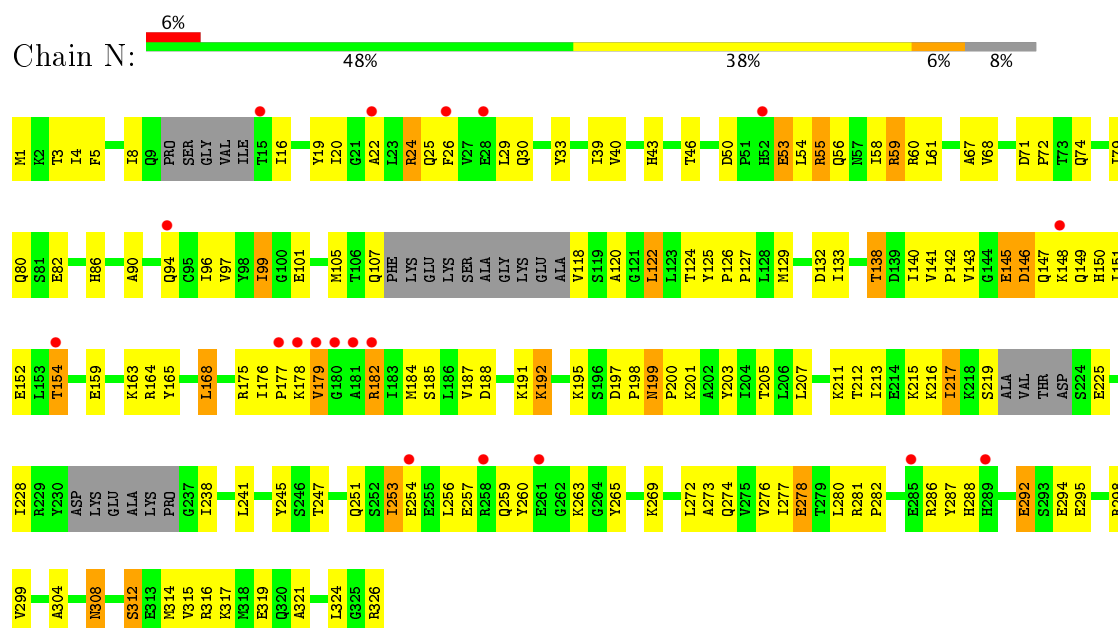




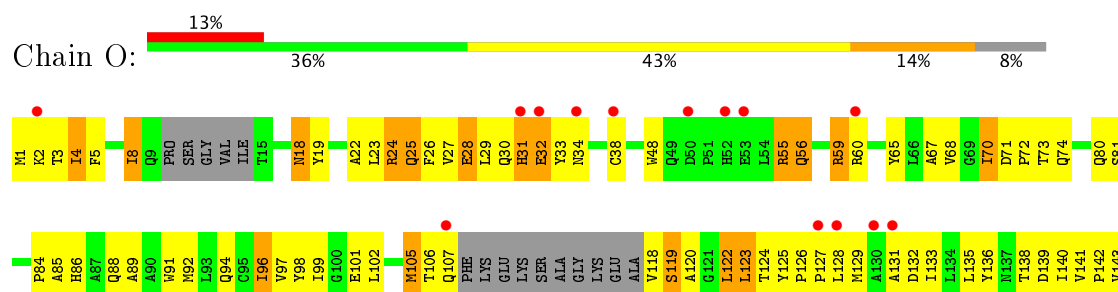
- Molecule 1: Tryptophanyl-tRNA synthetase



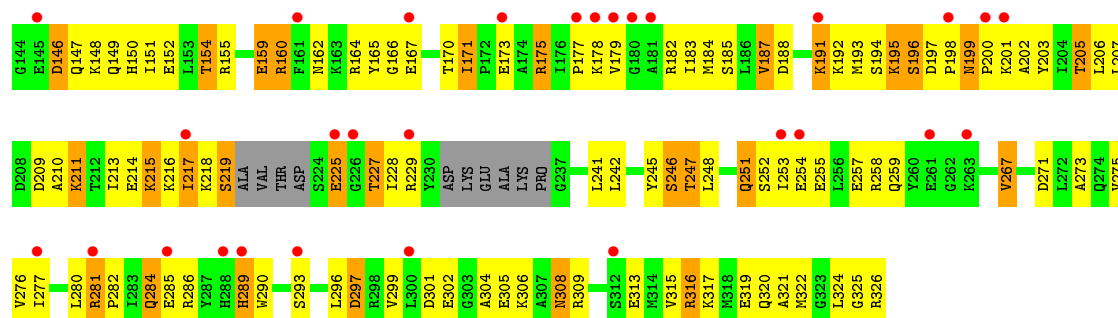
- Molecule 1: Tryptophanyl-tRNA synthetase



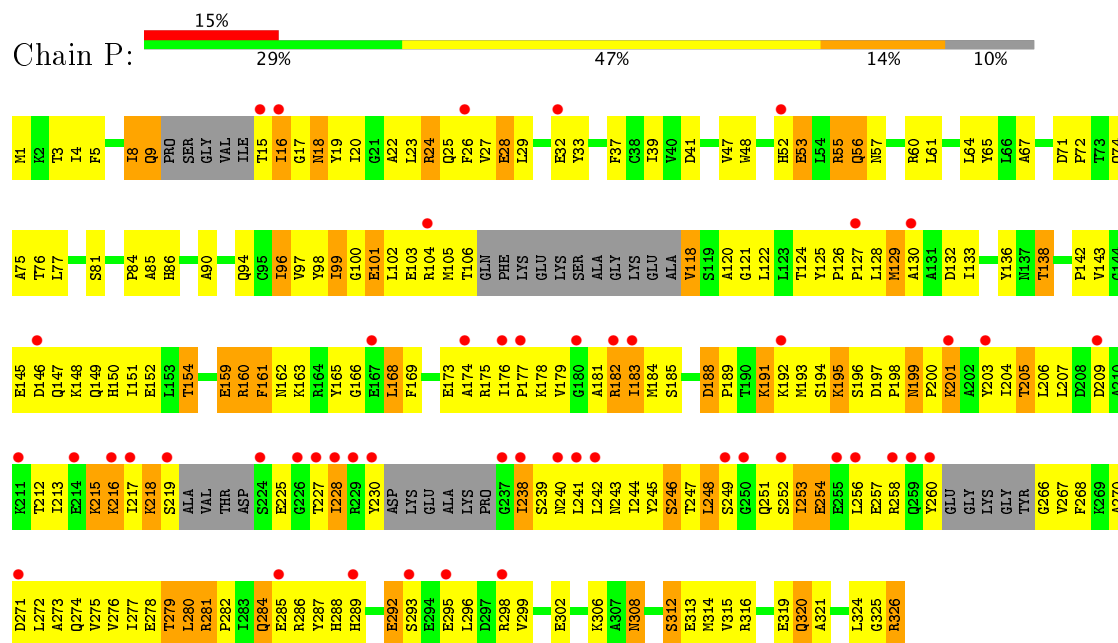
- Molecule 1: Tryptophanyl-tRNA synthetase



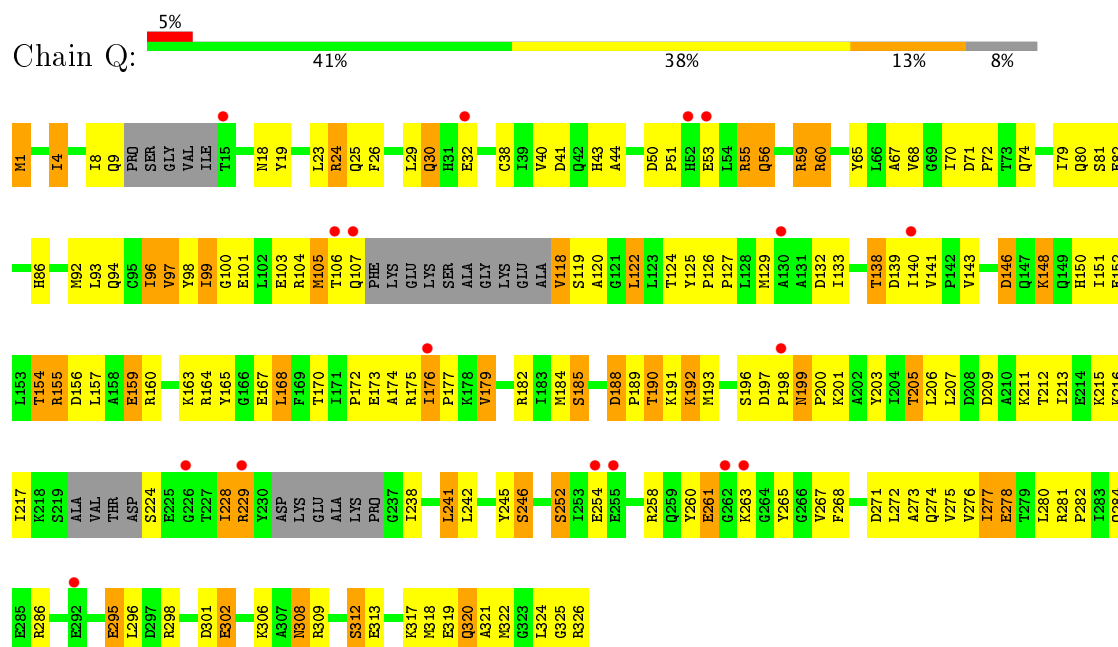




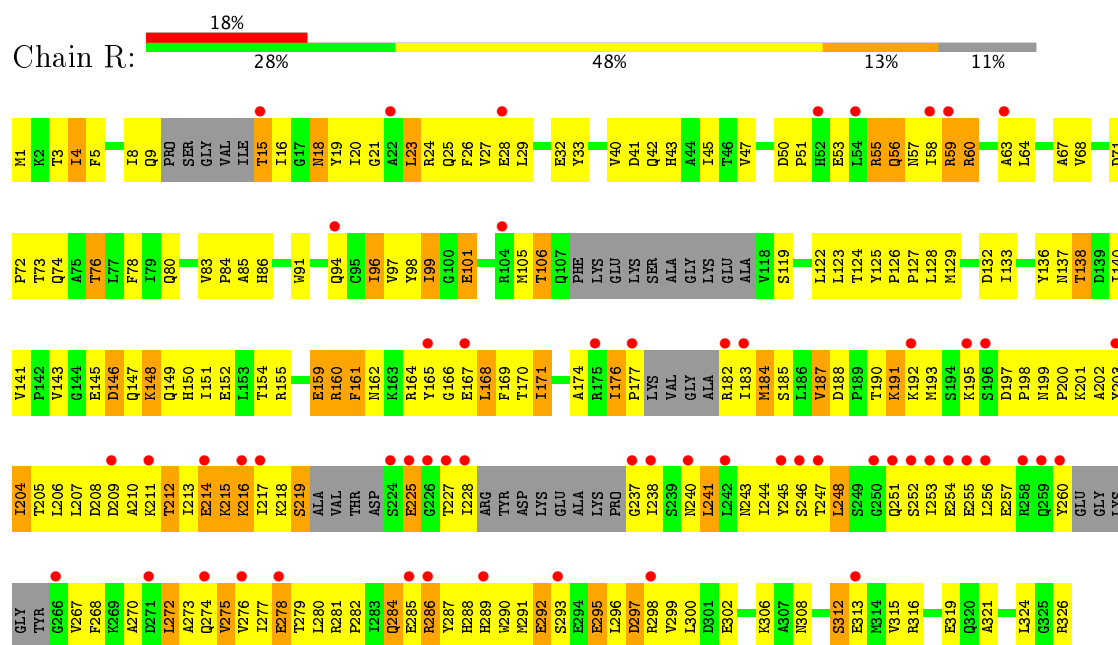
• Molecule 1: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase



● Molecule 1: Tryptophanyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.03Å 122.40Å 122.34Å 79.90° 80.52° 79.81°	Depositor
Resolution (Å)	25.00 – 2.70 24.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-2.70) 94.2 (24.96-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.220 0.250 , 0.264	Depositor DCC
$R_{free}$ test set	9240 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for l,h,k 0.048 for k,l,h 0.000 for -l,-k,-h 0.000 for -k,-h,-l 0.000 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	43727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.97 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.9719e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.38	0/2414	0.52	0/3242
1	B	0.30	0/2400	0.51	0/3222
1	C	0.31	0/2414	0.56	0/3242
1	D	0.32	0/2440	0.53	0/3278
1	E	0.29	0/2371	0.54	0/3184
1	F	0.29	0/2398	0.51	0/3219
1	G	0.30	0/2448	0.55	0/3289
1	H	0.29	0/2440	0.54	0/3278
1	I	0.31	0/2408	0.54	0/3235
1	J	0.30	0/2440	0.54	0/3278
1	K	0.28	0/2398	0.52	0/3220
1	L	0.31	0/2440	0.55	0/3278
1	M	0.28	0/2440	0.56	2/3278 (0.1%)
1	N	0.30	0/2440	0.56	0/3278
1	O	0.30	0/2440	0.56	0/3278
1	P	0.27	0/2391	0.57	1/3212 (0.0%)
1	Q	0.31	0/2440	0.57	1/3278 (0.0%)
1	R	0.29	0/2350	0.55	0/3156
All	All	0.30	0/43512	0.54	4/58445 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	44	ALA	CB-CA-C	-5.73	101.51	110.10
1	P	188	ASP	C-N-CD	-5.51	108.48	120.60
1	M	252	SER	N-CA-CB	-5.37	102.44	110.50
1	M	99	ILE	CB-CA-C	-5.31	100.98	111.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2383	0	2390	141	0
1	B	2370	0	2380	197	0
1	C	2383	0	2390	129	0
1	D	2408	0	2421	130	0
1	E	2342	0	2355	219	0
1	F	2368	0	2384	141	0
1	G	2416	0	2432	139	0
1	H	2408	0	2421	158	0
1	I	2377	0	2388	138	0
1	J	2408	0	2421	137	0
1	K	2367	0	2382	207	0
1	L	2408	0	2421	123	0
1	M	2408	0	2421	264	0
1	N	2408	0	2421	143	0
1	O	2408	0	2421	198	0
1	P	2361	0	2378	355	0
1	Q	2408	0	2421	172	0
1	R	2322	0	2333	283	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	2	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	9	0	0
2	G	15	0	9	2	0
2	H	15	0	9	1	0
2	I	15	0	9	0	0
2	J	15	0	9	2	0
2	K	15	0	9	0	0
2	L	15	0	9	0	0
2	M	15	0	9	0	0
2	N	15	0	9	0	0
2	O	15	0	9	0	0
2	P	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	15	0	9	1	0
2	R	15	0	9	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	3	0
3	F	5	0	0	2	0
3	G	5	0	0	1	0
3	H	5	0	0	2	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	1	0
3	L	5	0	0	0	0
3	M	5	0	0	3	0
3	N	5	0	0	2	0
3	O	5	0	0	2	0
3	P	5	0	0	7	0
3	Q	5	0	0	0	0
3	R	5	0	0	1	0
4	A	23	0	12	10	0
4	B	23	0	12	8	0
4	C	23	0	12	3	0
4	D	23	0	12	5	0
4	E	23	0	12	4	0
4	F	23	0	12	2	0
4	G	23	0	12	9	0
4	H	23	0	12	1	0
4	I	23	0	12	7	0
4	J	23	0	12	3	0
4	K	23	0	12	4	0
4	L	23	0	12	1	0
4	M	23	0	12	5	0
4	N	23	0	12	6	0
4	O	23	0	12	17	0
4	P	23	0	12	12	0
4	Q	23	0	12	7	0
4	R	23	0	12	4	0
All	All	43727	0	43558	3147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (3147) 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:Q:140:ILE:CD1	1:Q:175:ARG:HG3	1.54	1.36
1:M:23:LEU:HD21	1:M:65:TYR:CE1	1.72	1.24
1:I:199:ASN:ND2	1:I:200:PRO:HD2	1.54	1.23
1:Q:140:ILE:HD11	1:Q:175:ARG:CG	1.69	1.22
1:B:94:GLN:NE2	1:E:124:THR:HG21	1.55	1.20
1:I:199:ASN:HD22	1:I:200:PRO:CD	1.54	1.19
1:P:176:ILE:HB	1:P:179:VAL:CG2	1.71	1.18
1:M:105:MSE:CE	1:M:150:HIS:CE1	2.27	1.17
1:P:245:TYR:CE1	1:P:275:VAL:HG21	1.77	1.17
1:M:23:LEU:CD2	1:M:65:TYR:HE1	1.55	1.17
1:I:199:ASN:HD22	1:I:200:PRO:HD2	1.01	1.17
1:P:244:ILE:O	1:P:248:LEU:HD13	1.44	1.16
1:R:24:ARG:O	1:R:27:VAL:HG22	1.43	1.16
1:R:252:SER:OG	1:R:255:GLU:HB2	1.46	1.15
1:M:210:ALA:HB1	1:M:277:ILE:HD13	1.18	1.14
1:P:142:PRO:HA	1:P:175:ARG:O	1.46	1.14
1:K:245:TYR:CE2	1:K:256:LEU:HD11	1.83	1.14
1:M:23:LEU:CD2	1:M:65:TYR:CE1	2.28	1.14
1:P:151:ILE:HD13	1:P:174:ALA:HB2	1.16	1.14
1:I:205:THR:HG22	1:I:207:LEU:H	1.13	1.13
1:P:271:ASP:O	1:P:275:VAL:HG23	1.45	1.13
1:R:228:ILE:HG21	1:R:260:TYR:CB	1.79	1.13
1:K:260:TYR:HA	1:K:263:LYS:HD3	1.25	1.12
1:M:156:ASP:O	1:M:160:ARG:HG3	1.48	1.12
1:P:273:ALA:O	1:P:277:ILE:HG12	1.49	1.12
1:R:276:VAL:O	1:R:280:LEU:HG	1.47	1.12
1:E:20:ILE:HD12	1:E:20:ILE:H	1.02	1.12
1:K:245:TYR:CE1	1:K:275:VAL:HG11	1.86	1.10
1:P:281:ARG:HG3	1:P:282:PRO:HD3	1.23	1.10
1:O:5:PHE:HB2	1:O:138:THR:HG21	1.34	1.10
1:E:252:SER:OG	1:E:255:GLU:HB2	1.51	1.10
1:P:176:ILE:O	1:P:179:VAL:HG23	1.52	1.09
1:M:25:GLN:HG3	1:M:29:LEU:CD1	1.82	1.08
1:A:18:ASN:HD21	4:A:1003:AMP:H5'1	1.15	1.08
1:K:241:LEU:H	1:K:241:LEU:HD12	1.09	1.08
1:P:253:ILE:HG22	1:P:254:GLU:OE2	1.53	1.08
1:P:245:TYR:HB2	1:P:272:LEU:HD13	1.12	1.07
1:P:228:ILE:HG22	1:P:238:ILE:HD11	1.33	1.07
1:K:245:TYR:CD2	1:K:256:LEU:HD12	1.88	1.07
1:M:205:THR:HG22	1:M:207:LEU:H	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:253:ILE:HG22	1:P:254:GLU:CD	1.75	1.06
1:P:245:TYR:CB	1:P:272:LEU:HD13	1.85	1.06
1:E:136:TYR:OH	1:E:307:ALA:HB1	1.55	1.06
1:B:29:LEU:CD1	1:B:177:PRO:HB2	1.86	1.05
1:K:191:LYS:HD3	1:K:192:LYS:H	1.19	1.05
1:R:187:VAL:HG22	1:R:202:ALA:HB2	1.35	1.05
1:P:126:PRO:HG2	1:P:127:PRO:HD3	1.38	1.05
1:B:29:LEU:HD11	1:B:177:PRO:HB2	1.39	1.04
1:E:211:LYS:HD3	1:E:211:LYS:H	1.19	1.04
1:B:94:GLN:HE21	1:E:124:THR:HG21	0.94	1.03
1:P:100:GLY:O	1:P:104:ARG:HG3	1.57	1.03
1:G:188:ASP:OD1	1:G:190:THR:HG22	1.57	1.02
1:N:19:TYR:O	1:N:24:ARG:HB3	1.59	1.02
1:O:26:PHE:HD2	1:O:29:LEU:HD12	1.24	1.02
1:R:133:ILE:O	1:R:138:THR:HG23	1.59	1.02
1:I:24:ARG:HG2	1:I:24:ARG:HH11	1.19	1.02
1:C:205:THR:HG22	1:C:207:LEU:H	1.19	1.02
1:E:20:ILE:HD12	1:E:20:ILE:N	1.75	1.02
1:B:19:TYR:O	1:B:24:ARG:HB3	1.58	1.01
1:M:175:ARG:NH1	1:M:177:PRO:HG3	1.74	1.01
1:P:181:ALA:HB1	1:P:243:ASN:HD22	1.23	1.01
1:B:319:GLU:HB3	1:B:324:LEU:HB2	1.38	1.01
1:P:151:ILE:CD1	1:P:174:ALA:HB2	1.91	1.01
1:Q:140:ILE:CD1	1:Q:175:ARG:CG	2.32	1.00
1:K:124:THR:O	1:K:127:PRO:HD2	1.57	1.00
1:M:25:GLN:HG3	1:M:29:LEU:HD11	1.43	1.00
1:I:176:ILE:HG13	1:I:179:VAL:HG13	1.43	1.00
1:K:134:LEU:HB3	1:K:169:PHE:CD1	1.96	1.00
1:R:228:ILE:HB	1:R:260:TYR:O	1.58	1.00
1:R:260:TYR:CD1	1:R:268:PHE:HD1	1.79	1.00
1:I:258:ARG:O	1:I:261:GLU:HG2	1.60	1.00
1:H:274:GLN:O	1:H:278:GLU:HG2	1.62	1.00
1:P:24:ARG:HH22	1:P:247:THR:HB	1.22	1.00
1:K:134:LEU:HB3	1:K:169:PHE:CE1	1.98	0.99
1:J:258:ARG:HA	1:J:261:GLU:OE2	1.61	0.99
1:M:176:ILE:HB	1:M:179:VAL:HG12	1.44	0.99
1:M:199:ASN:ND2	1:M:201:LYS:HG2	1.75	0.99
1:R:187:VAL:HG22	1:R:202:ALA:CB	1.92	0.99
1:P:151:ILE:HD13	1:P:174:ALA:CB	1.94	0.98
1:K:245:TYR:CD2	1:K:256:LEU:CD1	2.46	0.98
1:H:205:THR:HG22	1:H:207:LEU:H	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:ASN:O	1:P:18:ASN:ND2	1.96	0.98
1:R:228:ILE:HG21	1:R:260:TYR:HB2	1.42	0.98
1:C:1:MSE:HG2	1:D:211:LYS:HD2	1.42	0.98
1:K:245:TYR:CE2	1:K:256:LEU:CD1	2.47	0.98
1:K:60:ARG:HA	1:K:291:MSE:HE1	1.45	0.97
1:M:161:PHE:CD2	1:M:169:PHE:HE2	1.82	0.97
1:M:280:LEU:O	1:M:284:GLN:HG3	1.65	0.97
1:E:20:ILE:H	1:E:20:ILE:CD1	1.78	0.97
1:O:26:PHE:CD2	1:O:29:LEU:HD12	1.99	0.97
1:P:29:LEU:O	1:P:33:TYR:HB2	1.65	0.96
1:F:107:GLN:HE21	1:F:107:GLN:H	1.09	0.96
1:M:105:MSE:HE2	1:M:150:HIS:CE1	1.97	0.96
1:R:228:ILE:HG21	1:R:260:TYR:HB3	1.46	0.96
1:K:237:GLY:O	1:K:241:LEU:HD11	1.65	0.96
1:R:279:THR:O	1:R:282:PRO:HD2	1.64	0.96
1:F:182:ARG:NH1	1:F:192:LYS:HD3	1.80	0.95
1:M:210:ALA:CB	1:M:277:ILE:HD13	1.95	0.95
1:P:16:ILE:HD11	1:P:193:MSE:HE1	1.48	0.95
1:M:159:GLU:O	1:M:163:LYS:HG3	1.66	0.95
1:M:26:PHE:HA	1:M:29:LEU:HB2	1.49	0.95
1:P:24:ARG:NH2	1:P:247:THR:HB	1.81	0.95
1:K:191:LYS:CD	1:K:192:LYS:H	1.79	0.95
1:M:225:GLU:HG2	1:M:227:THR:HG23	1.46	0.94
1:C:55:ARG:HH22	1:F:320:GLN:NE2	1.64	0.94
1:M:105:MSE:CE	1:M:150:HIS:ND1	2.30	0.94
1:A:124:THR:HG21	1:D:94:GLN:NE2	1.82	0.94
1:I:24:ARG:CG	1:I:24:ARG:HH11	1.81	0.94
1:M:105:MSE:HE1	1:M:150:HIS:ND1	1.82	0.94
1:R:251:GLN:HG3	1:R:256:LEU:HD11	1.45	0.94
1:F:107:GLN:NE2	1:F:107:GLN:H	1.66	0.94
1:K:191:LYS:HD3	1:K:192:LYS:N	1.82	0.94
1:P:176:ILE:HB	1:P:179:VAL:HG22	1.45	0.94
1:R:187:VAL:CG2	1:R:202:ALA:HB2	1.98	0.94
1:C:26:PHE:HA	1:C:29:LEU:HB2	1.47	0.93
1:H:254:GLU:O	1:H:258:ARG:HG3	1.68	0.93
1:B:137:ASN:HD21	1:B:314:MSE:HE1	1.30	0.93
1:P:239:SER:O	1:P:242:LEU:HB2	1.68	0.93
1:P:126:PRO:CG	1:P:127:PRO:HD3	1.99	0.93
1:M:161:PHE:HE2	1:M:168:LEU:HD23	1.31	0.92
1:G:18:ASN:HD21	4:G:1003:AMP:H5'2	1.34	0.92
1:O:18:ASN:HA	4:O:1003:AMP:H1'	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:254:GLU:HA	1:P:257:GLU:HB3	1.51	0.92
1:N:126:PRO:HB2	1:N:127:PRO:HD3	1.50	0.92
1:P:274:GLN:O	1:P:278:GLU:HG2	1.70	0.92
1:K:161:PHE:CE2	1:K:168:LEU:HD12	2.04	0.92
1:M:199:ASN:HD21	1:M:201:LYS:HG2	1.32	0.92
1:E:27:VAL:HG12	1:E:28:GLU:HG2	1.51	0.92
1:Q:205:THR:HG22	1:Q:207:LEU:H	1.31	0.92
1:P:124:THR:C	1:P:126:PRO:HD2	1.90	0.91
1:I:260:TYR:C	1:I:263:LYS:HG2	1.91	0.91
1:M:294:GLU:HG3	1:M:298:ARG:HH21	1.35	0.91
1:P:125:TYR:N	1:P:126:PRO:CD	2.33	0.91
1:K:125:TYR:N	1:K:126:PRO:CD	2.34	0.91
1:B:137:ASN:HD21	1:B:314:MSE:CE	1.84	0.91
1:R:165:TYR:HB3	1:R:321:ALA:HB1	1.52	0.91
1:R:185:SER:OG	1:R:202:ALA:HB1	1.69	0.91
1:E:184:MSE:HE3	1:E:191:LYS:C	1.91	0.90
1:K:25:GLN:O	1:K:29:LEU:HG	1.71	0.90
3:M:1002:PO4:O2	4:M:1003:AMP:H8	1.54	0.90
1:M:140:ILE:HG12	1:M:175:ARG:HB3	1.51	0.90
1:Q:94:GLN:O	1:Q:97:VAL:HG12	1.72	0.90
1:K:56:GLN:HE21	1:K:56:GLN:HA	1.35	0.90
1:R:213:ILE:HD12	1:R:277:ILE:HG12	1.53	0.90
1:M:126:PRO:HB2	1:M:127:PRO:HD3	1.51	0.89
1:M:209:ASP:OD1	1:M:212:THR:HB	1.73	0.89
1:N:245:TYR:HE2	1:N:256:LEU:CD2	1.84	0.89
1:R:252:SER:HG	1:R:255:GLU:HB2	1.37	0.89
1:A:320:GLN:HE21	1:D:55:ARG:NH2	1.70	0.89
1:N:205:THR:HG22	1:N:207:LEU:H	1.32	0.89
1:A:205:THR:HG22	1:A:207:LEU:H	1.36	0.89
1:R:211:LYS:O	1:R:215:LYS:HB2	1.73	0.89
1:P:245:TYR:CD2	1:P:256:LEU:HD13	2.07	0.88
1:E:205:THR:HG22	1:E:207:LEU:H	1.35	0.88
1:K:106:THR:H	1:K:149:GLN:HE22	1.13	0.88
1:N:308:ASN:O	1:N:312:SER:HB2	1.71	0.88
1:B:288:HIS:O	1:B:292:GLU:HG2	1.73	0.88
1:H:182:ARG:HG3	1:H:182:ARG:HH11	1.36	0.88
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.56	0.88
1:O:199:ASN:HD22	1:O:200:PRO:HD2	1.37	0.88
1:P:245:TYR:HD2	1:P:256:LEU:HD13	1.39	0.88
1:I:24:ARG:HG2	1:I:24:ARG:NH1	1.78	0.88
1:M:302:GLU:O	1:M:306:LYS:HG3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:176:ILE:O	1:N:179:VAL:HG22	1.72	0.88
1:H:308:ASN:O	1:H:312:SER:HB2	1.74	0.87
1:M:59:ARG:NH2	1:M:296:LEU:HD23	1.87	0.87
1:I:176:ILE:CG1	1:I:179:VAL:HG13	2.05	0.87
1:I:249:SER:OG	1:I:251:GLN:HG3	1.73	0.87
1:K:161:PHE:HE2	1:K:168:LEU:HD12	1.35	0.87
1:P:228:ILE:CG1	1:P:260:TYR:HB3	2.04	0.87
1:B:94:GLN:NE2	1:E:124:THR:CG2	2.37	0.87
1:E:211:LYS:HD3	1:E:211:LYS:N	1.88	0.87
1:E:98:TYR:HB2	1:E:101:GLU:HG3	1.57	0.87
1:H:56:GLN:HG2	1:H:60:ARG:CZ	2.04	0.87
1:M:161:PHE:CD2	1:M:169:PHE:CE2	2.61	0.87
1:R:225:GLU:OE2	1:R:227:THR:HG23	1.75	0.87
1:G:182:ARG:HG2	1:G:184:MSE:CE	2.05	0.86
1:M:282:PRO:HB2	1:M:286:ARG:HH21	1.40	0.86
1:E:30:GLN:HG3	1:E:74:GLN:HG2	1.57	0.86
1:N:50:ASP:HB3	1:N:53:GLU:HG2	1.58	0.86
1:D:19:TYR:O	1:D:24:ARG:HB2	1.75	0.86
1:E:241:LEU:HD22	1:E:241:LEU:N	1.89	0.86
1:K:159:GLU:OE2	1:K:163:LYS:HE3	1.76	0.86
1:P:245:TYR:HB2	1:P:272:LEU:CD1	2.03	0.86
1:R:105:MSE:HE1	1:R:150:HIS:HA	1.57	0.86
1:A:18:ASN:ND2	4:A:1003:AMP:H5'1	1.89	0.86
1:M:165:TYR:CE1	1:M:322:MSE:HA	2.09	0.86
1:R:308:ASN:O	1:R:312:SER:HB2	1.76	0.86
1:A:134:LEU:HB3	1:A:169:PHE:CD1	2.11	0.86
1:P:20:ILE:HD12	1:P:183:ILE:CD1	2.06	0.86
1:B:22:ALA:O	1:B:26:PHE:CD2	2.28	0.86
1:C:211:LYS:O	1:C:215:LYS:HG3	1.75	0.86
1:G:205:THR:HG22	1:G:207:LEU:H	1.41	0.86
1:E:19:TYR:HE1	1:E:68:VAL:HG13	1.41	0.86
1:F:25:GLN:O	1:F:29:LEU:HG	1.76	0.85
1:D:212:THR:HG22	1:D:216:LYS:HD2	1.58	0.85
1:P:181:ALA:HB1	1:P:243:ASN:ND2	1.90	0.85
1:H:199:ASN:ND2	1:H:201:LYS:H	1.74	0.85
1:N:24:ARG:HG2	1:N:24:ARG:HH11	1.42	0.85
1:P:228:ILE:CG2	1:P:238:ILE:HD11	2.06	0.85
1:K:141:VAL:HG12	1:K:143:VAL:HG13	1.59	0.85
1:E:280:LEU:O	1:E:284:GLN:HB2	1.76	0.85
1:A:320:GLN:NE2	1:D:55:ARG:NH2	2.24	0.85
1:P:121:GLY:O	1:P:125:TYR:HB3	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:GLU:HA	1:M:31:HIS:HD2	1.42	0.85
1:O:205:THR:HG22	1:O:207:LEU:H	1.41	0.85
1:B:2:LYS:H	1:B:2:LYS:HD2	1.41	0.85
1:G:171:ILE:HD13	1:G:171:ILE:N	1.92	0.85
1:F:22:ALA:O	1:F:26:PHE:CD2	2.30	0.85
1:O:205:THR:CG2	1:O:207:LEU:H	1.89	0.85
1:E:295:GLU:HG2	1:E:298:ARG:NH2	1.91	0.85
1:E:241:LEU:HD22	1:E:241:LEU:H	1.42	0.84
1:O:139:ASP:OD1	1:O:170:THR:HG21	1.77	0.84
1:R:29:LEU:O	1:R:33:TYR:HB2	1.75	0.84
1:E:30:GLN:HG3	1:E:74:GLN:CG	2.07	0.84
1:N:245:TYR:CE2	1:N:256:LEU:HD22	2.12	0.84
1:J:185:SER:HB3	1:J:188:ASP:O	1.78	0.84
1:M:182:ARG:HE	1:M:184:MSE:HE1	1.40	0.84
1:N:245:TYR:CE2	1:N:256:LEU:CD2	2.60	0.84
1:K:205:THR:HG22	1:K:207:LEU:H	1.43	0.84
1:P:125:TYR:N	1:P:126:PRO:HD2	1.90	0.84
1:I:99:ILE:HG12	1:L:118:VAL:O	1.75	0.84
1:R:213:ILE:CD1	1:R:277:ILE:HG12	2.08	0.84
1:R:282:PRO:O	1:R:286:ARG:HG3	1.77	0.84
1:R:16:ILE:O	1:R:20:ILE:HG12	1.76	0.84
1:M:165:TYR:CZ	1:M:322:MSE:HG2	2.12	0.84
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.57	0.84
1:C:316:ARG:HH21	1:C:316:ARG:HG3	1.42	0.83
1:I:99:ILE:CG1	1:L:118:VAL:O	2.26	0.83
1:H:176:ILE:O	1:H:179:VAL:HG22	1.78	0.83
1:I:199:ASN:HD22	1:I:200:PRO:N	1.76	0.83
1:M:143:VAL:HG21	1:M:151:ILE:HD11	1.60	0.83
1:M:164:ARG:NH1	1:P:48:TRP:CE2	2.46	0.83
1:G:171:ILE:H	1:G:171:ILE:HD13	1.42	0.83
1:M:23:LEU:HD22	1:M:65:TYR:CE1	2.11	0.83
1:B:320:GLN:NE2	1:E:55:ARG:NH2	2.27	0.83
1:N:22:ALA:O	1:N:26:PHE:CE2	2.31	0.83
1:P:272:LEU:O	1:P:276:VAL:HG23	1.79	0.83
1:Q:107:GLN:H	1:Q:107:GLN:NE2	1.76	0.83
1:K:124:THR:C	1:K:126:PRO:HD2	1.98	0.83
1:K:241:LEU:N	1:K:241:LEU:HD12	1.90	0.83
1:K:260:TYR:CA	1:K:263:LYS:HD3	2.07	0.83
1:L:281:ARG:HG3	1:L:281:ARG:HH11	1.41	0.83
1:M:94:GLN:O	1:P:120:ALA:HB3	1.79	0.83
1:O:118:VAL:HG12	1:R:99:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:GLU:HG3	1:G:317:LYS:NZ	1.94	0.83
1:K:260:TYR:HA	1:K:263:LYS:CD	2.06	0.83
1:K:245:TYR:HE1	1:K:275:VAL:HG11	1.42	0.83
1:M:161:PHE:CE2	1:M:168:LEU:HD23	2.14	0.83
1:J:101:GLU:O	1:J:105:MSE:CE	2.26	0.83
1:R:217:ILE:HD12	1:R:273:ALA:HA	1.60	0.82
1:I:205:THR:HG22	1:I:207:LEU:N	1.94	0.82
1:N:24:ARG:HG2	1:N:24:ARG:NH1	1.93	0.82
1:C:199:ASN:HD21	1:C:201:LYS:HB2	1.43	0.82
1:K:258:ARG:O	1:K:261:GLU:HG3	1.80	0.82
1:M:294:GLU:HG3	1:M:298:ARG:NH2	1.93	0.82
1:K:26:PHE:HA	1:K:29:LEU:HB2	1.61	0.82
1:M:165:TYR:HD1	1:M:321:ALA:O	1.62	0.82
1:G:126:PRO:HB2	1:G:127:PRO:HD3	1.58	0.82
1:J:18:ASN:O	1:J:23:LEU:HB2	1.79	0.82
1:M:118:VAL:O	1:P:98:TYR:HA	1.80	0.82
1:P:281:ARG:HG3	1:P:282:PRO:CD	2.08	0.82
1:J:98:TYR:HB2	1:J:101:GLU:HG3	1.62	0.82
1:M:64:LEU:CD2	1:M:287:TYR:CD1	2.61	0.82
1:N:245:TYR:HE2	1:N:256:LEU:HD21	1.44	0.82
1:E:245:TYR:O	1:E:249:SER:HB3	1.79	0.82
1:J:19:TYR:O	1:J:24:ARG:HB3	1.80	0.82
3:M:1002:PO4:O2	4:M:1003:AMP:C8	2.32	0.82
1:E:136:TYR:HH	1:E:307:ALA:HB1	1.41	0.82
1:G:288:HIS:O	1:G:292:GLU:HG2	1.78	0.82
1:E:267:VAL:HB	1:G:309:ARG:HH11	1.44	0.82
1:N:26:PHE:HA	1:N:29:LEU:HB2	1.60	0.82
1:M:241:LEU:HB3	1:M:268:PHE:HE2	1.45	0.81
1:B:175:ARG:HG3	1:B:176:ILE:N	1.93	0.81
1:N:50:ASP:HB3	1:N:53:GLU:CG	2.09	0.81
1:M:295:GLU:O	1:M:299:VAL:HG23	1.80	0.81
1:P:148:LYS:O	1:P:152:GLU:HG2	1.81	0.81
1:P:253:ILE:HB	1:P:254:GLU:OE1	1.80	0.81
1:P:281:ARG:N	1:P:282:PRO:HD2	1.96	0.81
1:B:260:TYR:OH	1:B:271:ASP:CB	2.28	0.81
1:I:22:ALA:O	1:I:26:PHE:CE2	2.34	0.81
1:P:295:GLU:HA	1:P:295:GLU:OE1	1.81	0.81
1:Q:281:ARG:HH11	1:Q:281:ARG:HG3	1.45	0.81
1:H:23:LEU:O	1:H:26:PHE:HB2	1.81	0.81
1:M:175:ARG:HH12	1:M:177:PRO:HG3	1.45	0.81
1:P:101:GLU:O	1:P:105:MSE:HG2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:TYR:HD1	1:N:272:LEU:HD13	1.42	0.81
1:M:176:ILE:HB	1:M:179:VAL:CG1	2.10	0.81
1:E:199:ASN:OD1	1:E:201:LYS:HG3	1.81	0.81
1:G:182:ARG:HG2	1:G:184:MSE:HE1	1.61	0.81
1:P:238:ILE:HD12	1:P:238:ILE:O	1.80	0.81
1:P:25:GLN:HG2	1:P:178:LYS:CB	2.11	0.81
1:O:175:ARG:HH22	1:O:177:PRO:CB	1.93	0.81
1:P:245:TYR:CB	1:P:272:LEU:CD1	2.58	0.81
1:R:205:THR:HG22	1:R:207:LEU:H	1.44	0.81
1:R:281:ARG:O	1:R:285:GLU:HG3	1.81	0.81
1:E:184:MSE:CE	1:E:191:LYS:C	2.50	0.80
1:H:23:LEU:O	1:H:23:LEU:HD12	1.80	0.80
1:M:199:ASN:HD22	1:M:200:PRO:HD2	1.47	0.80
1:P:19:TYR:O	1:P:24:ARG:HB2	1.82	0.80
1:A:124:THR:HG21	1:D:124:THR:HG21	1.63	0.80
1:C:98:TYR:HB2	1:C:101:GLU:HG3	1.63	0.80
1:M:282:PRO:CB	1:M:286:ARG:HH21	1.95	0.80
1:P:245:TYR:CE1	1:P:275:VAL:CG2	2.63	0.80
1:B:72:PRO:HB3	1:B:299:VAL:HG13	1.63	0.80
1:P:126:PRO:CD	1:P:127:PRO:CD	2.60	0.80
1:P:20:ILE:CD1	1:P:183:ILE:HD11	2.11	0.80
1:H:126:PRO:HB2	1:H:127:PRO:HD3	1.63	0.80
1:K:191:LYS:CD	1:K:192:LYS:N	2.42	0.80
1:P:193:MSE:HB3	4:P:1003:AMP:N6	1.96	0.80
1:O:26:PHE:O	1:O:30:GLN:HG3	1.82	0.80
1:P:143:VAL:HG21	1:P:151:ILE:HD11	1.64	0.80
1:P:247:THR:OG1	1:P:248:LEU:HD12	1.81	0.80
1:K:124:THR:O	1:K:127:PRO:CD	2.30	0.80
1:R:260:TYR:CE1	1:R:268:PHE:HD1	1.99	0.80
1:R:288:HIS:O	1:R:292:GLU:HG2	1.81	0.80
1:K:126:PRO:N	1:K:127:PRO:HD2	1.97	0.80
1:M:25:GLN:HG3	1:M:29:LEU:HD12	1.63	0.80
1:P:25:GLN:HG2	1:P:178:LYS:HB2	1.64	0.80
1:R:176:ILE:HG13	1:R:176:ILE:O	1.80	0.80
1:R:260:TYR:CD1	1:R:268:PHE:CD1	2.69	0.80
1:R:84:PRO:HD2	1:R:308:ASN:HD21	1.46	0.80
1:E:213:ILE:HD13	1:E:276:VAL:HG12	1.64	0.80
4:G:1003:AMP:H5'1	4:G:1003:AMP:H8	1.46	0.80
4:B:1003:AMP:C8	4:B:1003:AMP:H5'1	2.17	0.79
1:C:55:ARG:NH2	1:F:320:GLN:NE2	2.28	0.79
1:K:106:THR:H	1:K:149:GLN:NE2	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:LEU:HB3	1:F:169:PHE:CE1	2.16	0.79
4:A:1003:AMP:H8	4:A:1003:AMP:H5'1	1.47	0.79
1:J:205:THR:HG22	1:J:207:LEU:H	1.46	0.79
1:P:24:ARG:HG2	1:P:24:ARG:HH11	1.47	0.79
1:A:308:ASN:O	1:A:312:SER:HB2	1.83	0.79
1:H:176:ILE:HB	1:H:179:VAL:HG13	1.64	0.79
1:H:22:ALA:O	1:H:26:PHE:CD2	2.36	0.79
1:P:150:HIS:O	1:P:154:THR:HG23	1.81	0.79
1:R:260:TYR:CE1	1:R:268:PHE:CD1	2.71	0.79
4:K:1003:AMP:H5'1	4:K:1003:AMP:H8	1.48	0.79
1:R:20:ILE:HG13	1:R:183:ILE:HD12	1.64	0.79
1:C:205:THR:HG22	1:C:207:LEU:N	1.97	0.79
1:R:200:PRO:O	1:R:216:LYS:HE2	1.82	0.79
1:M:23:LEU:HD21	1:M:65:TYR:CZ	2.18	0.79
1:M:64:LEU:HD23	1:M:287:TYR:CD1	2.18	0.79
1:P:150:HIS:O	1:P:154:THR:CG2	2.30	0.79
1:C:320:GLN:NE2	1:F:55:ARG:NH2	2.31	0.79
1:N:29:LEU:HD11	1:N:177:PRO:HB2	1.65	0.79
1:P:248:LEU:HD12	1:P:248:LEU:N	1.97	0.79
1:P:24:ARG:CG	1:P:24:ARG:HH11	1.96	0.79
1:P:253:ILE:HG22	1:P:254:GLU:OE1	1.83	0.79
1:B:142:PRO:HA	1:B:175:ARG:O	1.81	0.78
1:E:280:LEU:HB3	1:E:284:GLN:OE1	1.83	0.78
1:M:281:ARG:HH11	1:M:281:ARG:HG2	1.46	0.78
1:Q:141:VAL:HG12	1:Q:143:VAL:HG13	1.65	0.78
1:R:199:ASN:OD1	1:R:201:LYS:HG2	1.83	0.78
1:B:254:GLU:H	1:B:254:GLU:CD	1.84	0.78
1:C:308:ASN:O	1:C:312:SER:HB2	1.83	0.78
1:D:98:TYR:HB2	1:D:101:GLU:HG3	1.66	0.78
1:G:98:TYR:HB2	1:G:101:GLU:HG3	1.65	0.78
1:P:24:ARG:HG2	1:P:24:ARG:NH1	1.97	0.78
1:K:125:TYR:N	1:K:126:PRO:HD3	1.97	0.78
1:P:126:PRO:CD	1:P:127:PRO:HD3	2.14	0.78
1:P:84:PRO:HD2	1:P:308:ASN:HD21	1.49	0.78
1:A:94:GLN:HE22	1:D:94:GLN:HE22	1.31	0.78
1:E:241:LEU:H	1:E:241:LEU:CD2	1.96	0.78
1:I:98:TYR:HB2	1:I:101:GLU:HG3	1.64	0.78
1:J:288:HIS:O	1:J:292:GLU:HG2	1.84	0.78
1:E:209:ASP:O	1:E:213:ILE:HG13	1.84	0.78
1:K:148:LYS:O	1:K:152:GLU:HG2	1.82	0.78
1:I:253:ILE:O	1:I:257:GLU:HG3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:302:GLU:O	1:O:306:LYS:HG3	1.83	0.78
1:Q:205:THR:CG2	1:Q:207:LEU:H	1.95	0.78
1:J:185:SER:CB	1:J:188:ASP:O	2.32	0.77
1:P:228:ILE:CG2	1:P:238:ILE:CD1	2.62	0.77
1:P:253:ILE:CB	1:P:254:GLU:OE1	2.32	0.77
1:M:211:LYS:HD3	1:Q:1:MSE:HG2	1.66	0.77
1:P:151:ILE:CD1	1:P:174:ALA:CB	2.56	0.77
1:P:253:ILE:CG2	1:P:254:GLU:OE1	2.32	0.77
1:R:290:TRP:HZ3	1:R:295:GLU:HB3	1.47	0.77
1:A:105:MSE:HE2	1:A:105:MSE:CA	2.14	0.77
1:E:267:VAL:HB	1:G:309:ARG:NH1	1.99	0.77
1:C:205:THR:CG2	1:C:207:LEU:H	1.94	0.77
1:H:98:TYR:HB2	1:H:101:GLU:HG3	1.67	0.77
1:P:182:ARG:O	1:P:184:MSE:HE2	1.85	0.77
1:G:295:GLU:HG3	1:G:298:ARG:HD3	1.66	0.77
1:I:126:PRO:HB2	1:I:127:PRO:HD3	1.66	0.77
1:I:55:ARG:NH2	1:L:320:GLN:NE2	2.33	0.77
1:P:281:ARG:N	1:P:282:PRO:CD	2.46	0.77
1:F:98:TYR:HB2	1:F:101:GLU:HG3	1.66	0.77
1:K:261:GLU:O	1:K:263:LYS:HD2	1.85	0.77
1:M:156:ASP:O	1:M:160:ARG:CG	2.31	0.77
1:P:205:THR:HG22	1:P:207:LEU:H	1.48	0.77
1:C:212:THR:HG22	1:C:216:LYS:HE3	1.67	0.76
1:K:259:GLN:HG3	1:K:260:TYR:N	2.00	0.76
1:J:126:PRO:HB2	1:J:127:PRO:HD3	1.68	0.76
1:M:165:TYR:CD1	1:M:321:ALA:O	2.38	0.76
1:R:184:MSE:H	1:R:240:ASN:HD21	1.33	0.76
1:B:199:ASN:HD21	1:B:201:LYS:HB2	1.50	0.76
1:B:205:THR:CG2	1:B:207:LEU:H	1.99	0.76
1:E:198:PRO:O	1:E:200:PRO:HD3	1.84	0.76
1:G:295:GLU:O	1:G:299:VAL:HG23	1.86	0.76
1:A:168:LEU:HD11	1:A:317:LYS:HD2	1.66	0.76
1:A:124:THR:HG21	1:D:94:GLN:HE22	1.48	0.76
1:H:27:VAL:O	1:H:31:HIS:CE1	2.38	0.76
1:L:19:TYR:O	1:L:24:ARG:HB3	1.84	0.76
1:R:19:TYR:CE2	1:R:24:ARG:HD2	2.19	0.76
1:B:187:VAL:HG22	1:B:202:ALA:HB2	1.68	0.76
1:A:141:VAL:HG12	1:A:143:VAL:HG13	1.66	0.76
1:E:284:GLN:O	1:E:288:HIS:CD2	2.38	0.76
1:Q:94:GLN:HA	1:Q:97:VAL:CG1	2.16	0.76
1:R:251:GLN:CG	1:R:256:LEU:HD11	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:PHE:CD1	1:D:37:PHE:HE2	2.04	0.76
1:P:279:THR:O	1:P:282:PRO:HD2	1.85	0.76
1:E:238:ILE:HA	1:E:241:LEU:HD23	1.67	0.76
1:K:210:ALA:O	1:K:214:GLU:HG3	1.85	0.76
1:R:126:PRO:HB2	1:R:127:PRO:HD3	1.66	0.76
1:J:187:VAL:CG2	1:J:202:ALA:HB2	2.16	0.76
1:P:288:HIS:O	1:P:292:GLU:HG3	1.85	0.76
1:P:244:ILE:O	1:P:248:LEU:CD1	2.30	0.76
1:F:182:ARG:NH2	1:F:192:LYS:HG3	2.00	0.75
1:H:199:ASN:C	1:H:199:ASN:HD22	1.89	0.75
1:G:225:GLU:OE1	1:I:163:LYS:HD3	1.86	0.75
1:K:245:TYR:HD2	1:K:256:LEU:HD12	1.45	0.75
1:F:185:SER:HB3	1:F:188:ASP:O	1.86	0.75
1:K:238:ILE:HA	1:K:241:LEU:HD11	1.68	0.75
1:L:8:ILE:HD13	1:L:65:TYR:CZ	2.21	0.75
1:O:182:ARG:O	1:O:184:MSE:HE2	1.87	0.75
1:O:98:TYR:HB2	1:O:101:GLU:HG3	1.68	0.75
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.69	0.75
1:M:98:TYR:HB2	1:M:101:GLU:HG3	1.68	0.75
1:N:24:ARG:CG	1:N:24:ARG:HH11	1.99	0.75
1:P:245:TYR:HA	1:P:272:LEU:CD1	2.16	0.75
1:R:145:GLU:O	1:R:145:GLU:HG2	1.86	0.75
1:R:41:ASP:HB3	1:R:58:ILE:HD11	1.66	0.75
1:G:18:ASN:HD21	4:G:1003:AMP:C5'	1.98	0.75
1:M:141:VAL:O	1:M:174:ALA:HA	1.85	0.75
4:N:1003:AMP:H5'2	4:N:1003:AMP:C8	2.22	0.75
1:O:38:CYS:SG	1:O:80:GLN:HB2	2.26	0.75
1:P:16:ILE:HG23	1:P:204:ILE:HB	1.68	0.75
1:A:79:ILE:HB	1:A:82:GLU:HG3	1.68	0.75
1:K:56:GLN:HA	1:K:56:GLN:NE2	2.01	0.75
1:L:126:PRO:HB2	1:L:127:PRO:HD3	1.68	0.75
1:P:176:ILE:HB	1:P:179:VAL:HG23	1.65	0.75
1:P:253:ILE:CG2	1:P:254:GLU:OE2	2.31	0.75
1:P:245:TYR:CA	1:P:272:LEU:CD1	2.65	0.75
1:B:29:LEU:HD13	1:B:177:PRO:HB2	1.68	0.75
1:F:249:SER:OG	1:F:251:GLN:HG3	1.86	0.75
1:L:308:ASN:O	1:L:312:SER:HB2	1.87	0.75
1:B:187:VAL:CG2	1:B:202:ALA:HB2	2.16	0.75
1:G:171:ILE:CD1	1:G:171:ILE:N	2.50	0.75
1:L:16:ILE:O	1:L:20:ILE:HG13	1.87	0.75
1:M:140:ILE:HG12	1:M:175:ARG:CB	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:TYR:HD2	1:N:256:LEU:HD13	1.50	0.75
1:O:140:ILE:CD1	1:O:175:ARG:HD3	2.17	0.75
1:H:151:ILE:HG21	1:H:174:ALA:HB2	1.68	0.74
1:P:126:PRO:N	1:P:127:PRO:HD2	2.02	0.74
1:R:184:MSE:H	1:R:240:ASN:ND2	1.85	0.74
1:A:243:ASN:O	1:A:247:THR:HG23	1.86	0.74
1:J:187:VAL:HG22	1:J:202:ALA:HB2	1.69	0.74
1:J:249:SER:OG	1:J:251:GLN:HG3	1.88	0.74
1:B:79:ILE:HB	1:B:82:GLU:HG3	1.68	0.74
1:F:205:THR:CG2	1:F:207:LEU:H	1.98	0.74
1:H:290:TRP:HZ3	1:H:295:GLU:HB3	1.53	0.74
1:A:124:THR:O	1:A:127:PRO:HD2	1.86	0.74
1:O:214:GLU:O	1:O:218:LYS:HG3	1.88	0.74
1:A:319:GLU:HB3	1:A:324:LEU:HB2	1.68	0.74
1:F:228:ILE:O	1:F:229:ARG:HG2	1.87	0.74
1:P:16:ILE:CG2	1:P:204:ILE:HB	2.17	0.74
1:M:165:TYR:HB3	1:M:321:ALA:HB1	1.69	0.74
1:Q:140:ILE:HD11	1:Q:175:ARG:O	1.87	0.74
1:R:225:GLU:CD	1:R:227:THR:HG23	2.08	0.74
1:K:124:THR:C	1:K:126:PRO:CD	2.56	0.74
1:I:124:THR:OG1	1:L:94:GLN:NE2	2.21	0.74
1:O:143:VAL:HG21	1:O:151:ILE:HD11	1.70	0.74
1:P:238:ILE:CD1	1:P:238:ILE:O	2.35	0.74
1:A:105:MSE:HE2	1:A:105:MSE:HA	1.68	0.74
1:K:15:THR:HA	1:K:204:ILE:O	1.88	0.74
1:D:246:SER:HB2	1:D:251:GLN:O	1.87	0.73
1:B:99:ILE:HD13	1:E:120:ALA:HA	1.69	0.73
1:P:126:PRO:N	1:P:127:PRO:CD	2.51	0.73
1:A:67:ALA:O	1:A:286:ARG:NH1	2.21	0.73
1:B:22:ALA:O	1:B:26:PHE:HD2	1.67	0.73
1:G:134:LEU:HB3	1:G:169:PHE:CD1	2.22	0.73
1:I:205:THR:CG2	1:I:207:LEU:H	1.98	0.73
1:I:308:ASN:O	1:I:312:SER:HB2	1.88	0.73
1:O:118:VAL:O	1:R:99:ILE:HG12	1.88	0.73
1:P:213:ILE:HD13	1:P:277:ILE:HD13	1.69	0.73
1:Q:211:LYS:O	1:Q:215:LYS:HG3	1.87	0.73
1:R:15:THR:HA	1:R:204:ILE:O	1.88	0.73
1:E:148:LYS:O	1:E:152:GLU:HG2	1.87	0.73
1:K:106:THR:N	1:K:149:GLN:HE22	1.84	0.73
1:M:105:MSE:HE3	1:M:150:HIS:CE1	2.23	0.73
1:Q:148:LYS:HD2	1:Q:152:GLU:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HA	1:C:31:HIS:HD2	1.54	0.73
1:F:107:GLN:N	1:F:107:GLN:HE21	1.85	0.73
1:B:8:ILE:HG22	1:B:61:LEU:HD21	1.70	0.73
1:G:205:THR:CG2	1:G:207:LEU:H	2.00	0.73
1:G:249:SER:OG	1:G:251:GLN:HG3	1.87	0.73
1:L:249:SER:OG	1:L:251:GLN:HG3	1.89	0.73
1:M:210:ALA:HB1	1:M:277:ILE:CD1	2.11	0.73
1:O:19:TYR:HE1	1:O:68:VAL:HG13	1.53	0.73
4:K:1003:AMP:H5'1	4:K:1003:AMP:C8	2.23	0.73
1:K:237:GLY:O	1:K:241:LEU:CD1	2.37	0.73
1:Q:209:ASP:O	1:Q:213:ILE:HG13	1.88	0.73
1:R:59:ARG:HD3	1:R:291:MSE:HE1	1.70	0.73
1:A:205:THR:HG22	1:A:207:LEU:N	2.04	0.73
1:B:137:ASN:ND2	1:B:314:MSE:CE	2.51	0.73
1:E:120:ALA:O	1:E:124:THR:HG23	1.88	0.73
1:J:101:GLU:O	1:J:105:MSE:HE1	1.88	0.73
1:J:146:ASP:OD1	1:J:146:ASP:N	2.22	0.73
1:N:212:THR:HG22	1:N:216:LYS:HD2	1.70	0.73
1:H:134:LEU:HB3	1:H:169:PHE:CD1	2.24	0.72
1:D:249:SER:OG	1:D:251:GLN:HG3	1.89	0.72
1:A:22:ALA:O	1:A:25:GLN:HG2	1.89	0.72
1:G:41:ASP:OD2	1:G:81:SER:HB3	1.88	0.72
1:I:249:SER:CB	1:I:251:GLN:HG3	2.19	0.72
1:I:260:TYR:CA	1:I:263:LYS:HG2	2.18	0.72
1:K:188:ASP:OD1	1:K:190:THR:HB	1.88	0.72
1:R:272:LEU:HD12	1:R:272:LEU:O	1.89	0.72
1:C:55:ARG:NH2	1:F:320:GLN:HE22	1.87	0.72
1:D:25:GLN:O	1:D:29:LEU:HG	1.88	0.72
1:E:56:GLN:HB3	1:E:60:ARG:NH2	2.04	0.72
1:P:100:GLY:O	1:P:104:ARG:CG	2.37	0.72
1:P:228:ILE:HG23	1:P:238:ILE:HD13	1.70	0.72
1:B:187:VAL:HG22	1:B:202:ALA:CB	2.18	0.72
1:C:199:ASN:ND2	1:C:201:LYS:H	1.87	0.72
1:D:205:THR:HG22	1:D:207:LEU:H	1.54	0.72
1:J:256:LEU:HD23	1:J:259:GLN:NE2	2.04	0.72
1:P:289:HIS:O	1:P:293:SER:CB	2.37	0.72
1:M:54:LEU:O	1:M:58:ILE:HG13	1.88	0.72
1:H:205:THR:HG22	1:H:207:LEU:N	2.02	0.72
1:M:185:SER:OG	1:M:187:VAL:HG23	1.90	0.72
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.54	0.72
1:G:309:ARG:HB3	1:G:309:ARG:CZ	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLN:HG2	1:H:60:ARG:NH2	2.05	0.72
1:P:289:HIS:O	1:P:293:SER:HB3	1.90	0.72
1:Q:157:LEU:CD2	1:Q:160:ARG:NH2	2.52	0.72
1:J:184:MSE:HB3	1:J:189:PRO:O	1.88	0.72
1:A:205:THR:CG2	1:A:207:LEU:H	2.01	0.72
1:L:162:ASN:HA	1:L:166:GLY:O	1.90	0.72
1:P:118:VAL:HG12	1:P:122:LEU:CD1	2.20	0.72
1:H:243:ASN:O	1:H:247:THR:HG23	1.90	0.71
1:I:258:ARG:HA	1:I:261:GLU:OE2	1.90	0.71
1:J:308:ASN:O	1:J:312:SER:HB2	1.90	0.71
1:J:8:ILE:HD12	1:J:65:TYR:OH	1.90	0.71
1:D:67:ALA:O	1:D:286:ARG:NH1	2.24	0.71
1:J:205:THR:CG2	1:J:207:LEU:H	2.02	0.71
1:M:134:LEU:HB3	1:M:169:PHE:CE1	2.25	0.71
1:N:120:ALA:HB3	1:Q:97:VAL:CG1	2.20	0.71
1:M:195:LYS:HG2	3:M:1002:PO4:O3	1.90	0.71
1:O:3:THR:HG22	1:O:138:THR:HG22	1.71	0.71
1:E:105:MSE:HA	1:E:105:MSE:HE2	1.72	0.71
1:F:182:ARG:CZ	1:F:192:LYS:HG3	2.21	0.71
1:Q:100:GLY:O	1:Q:104:ARG:HG3	1.90	0.71
1:E:211:LYS:H	1:E:211:LYS:CD	2.02	0.71
1:P:238:ILE:O	1:P:238:ILE:CG1	2.37	0.71
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.72	0.71
1:L:5:PHE:HB2	1:L:138:THR:HG21	1.73	0.71
1:P:16:ILE:HG12	1:P:17:GLY:N	2.04	0.71
1:Q:126:PRO:HB2	1:Q:127:PRO:HD3	1.72	0.71
1:E:211:LYS:N	1:E:211:LYS:CD	2.52	0.71
1:F:141:VAL:HG12	1:F:143:VAL:HG13	1.71	0.71
1:K:241:LEU:H	1:K:241:LEU:CD1	1.87	0.71
1:L:243:ASN:O	1:L:247:THR:HG23	1.90	0.71
1:M:281:ARG:O	1:M:285:GLU:HB2	1.91	0.71
1:A:249:SER:OG	1:A:251:GLN:HG3	1.90	0.71
1:G:175:ARG:O	1:G:177:PRO:HD3	1.91	0.71
1:G:19:TYR:HA	1:G:23:LEU:HB3	1.72	0.71
1:O:8:ILE:HD12	1:O:65:TYR:OH	1.90	0.71
1:R:86:HIS:HD2	1:R:132:ASP:OD1	1.74	0.71
1:G:133:ILE:O	1:G:138:THR:HG23	1.90	0.71
1:G:271:ASP:OD1	1:K:309:ARG:NH1	2.23	0.71
1:M:120:ALA:HB2	1:P:102:LEU:HD12	1.73	0.71
1:B:199:ASN:ND2	1:B:201:LYS:HB2	2.05	0.71
1:B:230:TYR:CE1	1:B:239:SER:HB3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LYS:HG3	1:E:149:GLN:H	1.56	0.71
1:G:96:ILE:O	1:G:160:ARG:NH1	2.24	0.71
1:Q:151:ILE:O	1:Q:155:ARG:HG3	1.91	0.71
1:Q:157:LEU:HD23	1:Q:160:ARG:NH2	2.06	0.71
1:A:71:ASP:OD1	1:A:73:THR:HG23	1.91	0.70
1:M:25:GLN:CG	1:M:29:LEU:HD11	2.20	0.70
1:A:94:GLN:NE2	1:D:94:GLN:HE22	1.89	0.70
1:H:15:THR:HB	1:H:204:ILE:O	1.91	0.70
1:C:243:ASN:O	1:C:247:THR:HG23	1.91	0.70
1:F:19:TYR:CE2	1:F:24:ARG:HD2	2.26	0.70
1:Q:140:ILE:HD12	1:Q:175:ARG:CG	2.19	0.70
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.71	0.70
1:F:315:VAL:O	1:F:319:GLU:HG3	1.90	0.70
1:H:182:ARG:HH11	1:H:182:ARG:CG	2.03	0.70
1:H:67:ALA:O	1:H:286:ARG:NH1	2.24	0.70
1:M:5:PHE:HB2	1:M:138:THR:HG21	1.72	0.70
1:B:96:ILE:O	1:B:160:ARG:NH1	2.24	0.70
1:I:18:ASN:HD21	4:I:1003:AMP:H5'2	1.56	0.70
1:B:150:HIS:O	1:B:154:THR:HG22	1.92	0.70
1:J:273:ALA:O	1:J:277:ILE:HD12	1.92	0.70
1:M:319:GLU:HG2	1:M:324:LEU:HD12	1.72	0.70
1:D:133:ILE:O	1:D:138:THR:HG23	1.92	0.70
1:C:320:GLN:NE2	1:F:55:ARG:HH22	1.90	0.70
1:K:238:ILE:O	1:K:241:LEU:CD1	2.39	0.70
1:K:98:TYR:HB2	1:K:101:GLU:HG3	1.73	0.70
1:O:326:ARG:HH12	1:R:300:LEU:HB2	1.57	0.70
1:Q:205:THR:HG22	1:Q:207:LEU:N	2.06	0.70
1:H:99:ILE:O	1:H:103:GLU:HG3	1.92	0.70
1:H:199:ASN:HD22	1:H:201:LYS:H	1.39	0.70
1:M:199:ASN:HD22	1:M:200:PRO:CD	2.04	0.70
1:P:241:LEU:HD23	1:P:244:ILE:HD12	1.72	0.70
1:P:228:ILE:HG13	1:P:260:TYR:HB3	1.73	0.70
1:E:184:MSE:HE3	1:E:191:LYS:N	2.06	0.70
1:E:184:MSE:HE3	1:E:191:LYS:O	1.91	0.70
1:M:214:GLU:O	1:M:218:LYS:HG3	1.91	0.70
1:M:282:PRO:HB2	1:M:286:ARG:NH2	2.06	0.70
1:N:245:TYR:CD1	1:N:272:LEU:HD13	2.25	0.70
1:P:15:THR:HA	1:P:204:ILE:O	1.92	0.70
1:R:129:MSE:O	1:R:132:ASP:HB2	1.91	0.70
1:M:94:GLN:OE1	1:M:124:THR:HB	1.92	0.70
1:P:213:ILE:CD1	1:P:277:ILE:HD13	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:308:ASN:O	1:M:312:SER:HB2	1.91	0.69
4:N:1003:AMP:H5'2	4:N:1003:AMP:H8	1.56	0.69
1:P:20:ILE:HD13	1:P:183:ILE:HD11	1.73	0.69
1:R:290:TRP:CZ3	1:R:295:GLU:HB3	2.26	0.69
1:E:184:MSE:SE	1:E:192:LYS:HA	2.43	0.69
1:G:273:ALA:O	1:G:277:ILE:HD12	1.92	0.69
1:H:29:LEU:CD1	1:H:177:PRO:HB2	2.22	0.69
1:P:67:ALA:O	1:P:286:ARG:NH1	2.25	0.69
1:E:245:TYR:CA	1:E:272:LEU:HD13	2.22	0.69
1:J:120:ALA:O	1:J:124:THR:CG2	2.40	0.69
1:B:199:ASN:HD22	1:B:200:PRO:HD2	1.57	0.69
1:O:105:MSE:HA	1:O:105:MSE:HE2	1.73	0.69
1:P:122:LEU:O	1:P:125:TYR:CD1	2.46	0.69
1:M:214:GLU:OE1	1:Q:1:MSE:HE2	1.92	0.69
1:C:22:ALA:O	1:C:26:PHE:CE2	2.45	0.69
1:G:165:TYR:HB3	1:G:321:ALA:HB1	1.73	0.69
1:K:3:THR:HB	1:K:138:THR:HA	1.73	0.69
1:M:205:THR:HG22	1:M:207:LEU:N	1.99	0.69
1:R:19:TYR:HE1	1:R:68:VAL:HG13	1.57	0.69
1:A:280:LEU:O	1:A:284:GLN:HG3	1.93	0.69
1:C:55:ARG:HH22	1:F:320:GLN:HE22	1.40	0.69
1:E:27:VAL:CG1	1:E:28:GLU:HG2	2.21	0.69
1:B:137:ASN:HA	1:B:170:THR:HG23	1.74	0.69
1:B:205:THR:HG23	1:B:207:LEU:H	1.58	0.69
1:K:25:GLN:O	1:K:29:LEU:CG	2.40	0.69
1:K:79:ILE:HB	1:K:82:GLU:HG3	1.74	0.69
1:L:273:ALA:O	1:L:277:ILE:HG13	1.93	0.69
1:O:120:ALA:HA	1:R:99:ILE:HD13	1.74	0.69
1:P:241:LEU:HD22	1:P:272:LEU:CD2	2.23	0.69
1:I:150:HIS:O	1:I:154:THR:HG23	1.93	0.69
1:K:281:ARG:N	1:K:282:PRO:HD2	2.08	0.69
1:M:199:ASN:ND2	1:M:200:PRO:HD2	2.07	0.69
1:O:27:VAL:O	1:O:30:GLN:NE2	2.24	0.69
1:O:315:VAL:O	1:O:319:GLU:HG3	1.92	0.69
1:R:253:ILE:O	1:R:257:GLU:HB2	1.92	0.69
1:E:225:GLU:HG2	1:E:225:GLU:O	1.91	0.69
1:I:133:ILE:O	1:I:138:THR:HG23	1.92	0.69
1:H:99:ILE:HG13	1:K:118:VAL:HB	1.74	0.69
1:K:295:GLU:HG2	1:K:298:ARG:NH1	2.07	0.69
1:G:224:SER:HB3	1:I:166:GLY:HA2	1.74	0.69
1:R:228:ILE:CB	1:R:260:TYR:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.58	0.69
1:B:72:PRO:HB3	1:B:299:VAL:CG1	2.22	0.69
1:P:145:GLU:CD	1:P:145:GLU:H	1.96	0.69
1:P:56:GLN:OE1	1:P:60:ARG:NH2	2.26	0.69
1:Q:260:TYR:O	1:Q:263:LYS:HB2	1.93	0.69
1:R:273:ALA:O	1:R:277:ILE:HG13	1.93	0.69
1:R:291:MSE:HE3	1:R:291:MSE:O	1.93	0.69
1:H:150:HIS:O	1:H:154:THR:HG22	1.93	0.68
1:K:238:ILE:O	1:K:241:LEU:HD13	1.93	0.68
1:O:175:ARG:HH22	1:O:177:PRO:CA	2.06	0.68
1:M:281:ARG:CG	1:M:281:ARG:HH11	2.05	0.68
1:R:165:TYR:CD2	1:R:321:ALA:O	2.46	0.68
1:R:252:SER:OG	1:R:255:GLU:CB	2.36	0.68
1:D:315:VAL:O	1:D:319:GLU:HG3	1.93	0.68
1:K:287:TYR:OH	1:K:291:MSE:HE3	1.93	0.68
1:M:23:LEU:HD21	1:M:65:TYR:HE1	1.16	0.68
1:R:208:ASP:OD2	1:R:216:LYS:NZ	2.25	0.68
1:F:175:ARG:O	1:F:175:ARG:HG3	1.94	0.68
1:J:120:ALA:O	1:J:124:THR:HG23	1.94	0.68
1:O:147:GLN:O	1:O:151:ILE:HG12	1.94	0.68
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.28	0.68
1:I:185:SER:HB3	1:I:188:ASP:O	1.93	0.68
1:K:280:LEU:O	1:K:284:GLN:HG3	1.93	0.68
1:H:260:TYR:HD1	1:H:263:LYS:HG3	1.59	0.68
1:H:290:TRP:CZ3	1:H:295:GLU:HB3	2.28	0.68
1:R:98:TYR:HB2	1:R:101:GLU:HG3	1.73	0.68
1:K:20:ILE:HD12	1:K:183:ILE:HG13	1.76	0.68
1:M:185:SER:HG	1:M:187:VAL:HG23	1.59	0.68
1:A:124:THR:CG2	1:D:94:GLN:NE2	2.57	0.68
1:B:151:ILE:HA	1:B:154:THR:HG23	1.76	0.68
1:B:71:ASP:HB3	1:B:74:GLN:HB3	1.75	0.68
1:E:252:SER:OG	1:E:255:GLU:CB	2.35	0.68
1:M:200:PRO:HA	1:M:203:TYR:CE2	2.28	0.68
1:P:122:LEU:O	1:P:125:TYR:HD1	1.77	0.68
1:R:272:LEU:HA	1:R:275:VAL:CG1	2.24	0.68
1:B:155:ARG:NH1	1:B:172:PRO:O	2.27	0.68
1:F:134:LEU:HB3	1:F:169:PHE:CD1	2.29	0.68
1:G:193:MSE:HB3	4:G:1003:AMP:HN62	1.59	0.68
1:K:125:TYR:CD1	1:K:126:PRO:HD3	2.29	0.68
1:K:318:MSE:O	1:K:322:MSE:HG3	1.93	0.68
1:N:67:ALA:O	1:N:286:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:71:ASP:OD2	1:O:74:GLN:N	2.27	0.68
1:E:205:THR:HG22	1:E:207:LEU:N	2.09	0.68
1:R:43:HIS:CE1	1:R:80:GLN:HE22	2.11	0.68
1:H:137:ASN:HD22	1:H:170:THR:HG23	1.59	0.67
1:K:105:MSE:CE	1:K:150:HIS:ND1	2.57	0.67
1:B:304:ALA:O	1:B:308:ASN:HB2	1.95	0.67
1:C:22:ALA:O	1:C:26:PHE:CD2	2.48	0.67
1:C:29:LEU:HD22	1:C:33:TYR:CE1	2.29	0.67
1:D:23:LEU:HD13	1:D:65:TYR:CZ	2.30	0.67
1:H:27:VAL:O	1:H:31:HIS:HE1	1.77	0.67
1:J:67:ALA:O	1:J:286:ARG:NH1	2.27	0.67
1:M:261:GLU:O	1:M:263:LYS:HG2	1.94	0.67
1:E:188:ASP:OD1	1:E:190:THR:HG23	1.94	0.67
1:H:29:LEU:HD13	1:H:177:PRO:HB2	1.76	0.67
1:M:165:TYR:HE1	1:M:322:MSE:HA	1.54	0.67
1:N:217:ILE:O	1:N:269:LYS:HE2	1.94	0.67
1:R:218:LYS:HG2	1:R:219:SER:N	2.10	0.67
1:E:245:TYR:CB	1:E:272:LEU:HD13	2.24	0.67
1:M:207:LEU:HD11	1:M:287:TYR:CZ	2.29	0.67
1:N:245:TYR:HD2	1:N:256:LEU:CD1	2.07	0.67
1:P:267:VAL:O	1:P:271:ASP:N	2.27	0.67
1:B:305:GLU:O	1:B:309:ARG:HG3	1.95	0.67
1:D:8:ILE:HD12	1:D:65:TYR:OH	1.94	0.67
1:E:148:LYS:HG3	1:E:149:GLN:N	2.10	0.67
1:N:16:ILE:O	1:N:20:ILE:HG13	1.95	0.67
4:P:1003:AMP:H5'2	4:P:1003:AMP:C4	2.28	0.67
1:Q:176:ILE:O	1:Q:176:ILE:HG13	1.91	0.67
1:R:214:GLU:HB3	1:R:273:ALA:HB1	1.76	0.67
1:F:151:ILE:HD13	1:F:151:ILE:N	2.10	0.67
1:J:41:ASP:OD2	1:J:81:SER:HB3	1.94	0.67
1:M:134:LEU:HB3	1:M:169:PHE:CD1	2.30	0.67
1:M:278:GLU:OE1	1:M:281:ARG:NH2	2.26	0.67
1:O:193:MSE:HB3	4:O:1003:AMP:N6	2.10	0.67
1:R:147:GLN:O	1:R:150:HIS:HB2	1.94	0.67
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.30	0.67
1:D:19:TYR:HA	1:D:23:LEU:HB3	1.76	0.67
1:A:320:GLN:NE2	1:D:55:ARG:HH22	1.90	0.67
1:N:273:ALA:O	1:N:277:ILE:HD12	1.95	0.67
1:P:245:TYR:HD2	1:P:256:LEU:CD1	2.08	0.67
1:R:199:ASN:OD1	1:R:201:LYS:CG	2.43	0.67
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:LEU:HD21	1:D:314:MSE:SE	2.45	0.67
1:E:133:ILE:HD13	1:E:141:VAL:HG21	1.77	0.67
1:N:245:TYR:CE2	1:N:256:LEU:HD21	2.26	0.67
1:J:193:MSE:HB3	4:J:1003:AMP:HN62	1.60	0.67
1:L:313:GLU:HG3	1:L:317:LYS:NZ	2.09	0.67
1:R:206:LEU:O	1:R:207:LEU:HD23	1.95	0.67
1:B:320:GLN:NE2	1:E:55:ARG:HH22	1.91	0.67
1:L:319:GLU:HB3	1:L:324:LEU:HB2	1.77	0.67
1:M:188:ASP:OD2	1:M:190:THR:HB	1.95	0.67
1:R:25:GLN:H	1:R:25:GLN:CD	1.97	0.67
1:E:185:SER:HB3	1:E:188:ASP:O	1.95	0.66
1:H:313:GLU:OE2	1:H:316:ARG:NH1	2.28	0.66
1:I:214:GLU:O	1:I:218:LYS:HG3	1.96	0.66
1:M:84:PRO:O	1:M:88:GLN:HG3	1.96	0.66
1:N:22:ALA:O	1:N:26:PHE:HE2	1.77	0.66
1:Q:308:ASN:O	1:Q:312:SER:HB2	1.94	0.66
1:C:199:ASN:HD22	1:C:201:LYS:H	1.44	0.66
1:L:199:ASN:HD22	1:L:200:PRO:HD2	1.60	0.66
1:M:28:GLU:HA	1:M:31:HIS:CD2	2.27	0.66
1:P:90:ALA:HB2	1:P:128:LEU:HD12	1.76	0.66
1:P:20:ILE:HD12	1:P:183:ILE:HD12	1.75	0.66
1:R:19:TYR:CD2	1:R:24:ARG:HD2	2.31	0.66
1:R:272:LEU:HA	1:R:275:VAL:HG12	1.76	0.66
1:B:255:GLU:HA	1:B:258:ARG:HH21	1.60	0.66
1:P:209:ASP:OD1	1:P:212:THR:HB	1.95	0.66
1:P:238:ILE:O	1:P:238:ILE:HG13	1.95	0.66
1:M:188:ASP:OD1	1:M:190:THR:HB	1.95	0.66
1:B:188:ASP:OD1	1:B:190:THR:HB	1.94	0.66
1:E:314:MSE:O	1:E:318:MSE:HG3	1.95	0.66
1:F:67:ALA:O	1:F:286:ARG:NH1	2.28	0.66
1:J:193:MSE:O	4:J:1003:AMP:N6	2.28	0.66
1:M:188:ASP:CG	1:M:190:THR:HB	2.16	0.66
1:P:245:TYR:HD1	1:P:272:LEU:HD12	1.60	0.66
1:R:199:ASN:OD1	1:R:201:LYS:N	2.26	0.66
1:R:23:LEU:O	1:R:26:PHE:HB2	1.95	0.66
1:A:193:MSE:HB3	4:A:1003:AMP:HN62	1.61	0.66
1:B:272:LEU:HA	1:B:275:VAL:HG13	1.77	0.66
1:C:199:ASN:ND2	1:C:201:LYS:HB2	2.09	0.66
1:E:79:ILE:HB	1:E:82:GLU:HG3	1.76	0.66
1:G:71:ASP:O	1:G:75:ALA:N	2.27	0.66
1:J:141:VAL:HG12	1:J:143:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:94:GLN:HA	1:Q:97:VAL:HG12	1.77	0.66
1:R:72:PRO:HB3	1:R:299:VAL:HG13	1.78	0.66
1:B:288:HIS:O	1:B:292:GLU:CG	2.44	0.66
1:G:260:TYR:HA	1:G:263:LYS:HG3	1.77	0.66
1:J:57:ASN:OD1	1:J:60:ARG:NH2	2.28	0.66
1:M:32:GLU:O	1:M:32:GLU:HG3	1.93	0.66
1:Q:302:GLU:O	1:Q:306:LYS:HG3	1.95	0.66
1:R:5:PHE:HB2	1:R:138:THR:HG21	1.78	0.66
1:R:270:ALA:O	1:R:273:ALA:HB3	1.96	0.66
1:E:281:ARG:HB3	1:E:282:PRO:HD3	1.78	0.66
1:F:29:LEU:CD1	1:F:177:PRO:HB2	2.25	0.66
1:G:324:LEU:O	1:J:55:ARG:NH1	2.28	0.66
1:I:67:ALA:O	1:I:286:ARG:NH1	2.28	0.66
1:M:98:TYR:CE2	1:M:160:ARG:NH2	2.64	0.66
1:N:94:GLN:O	1:N:97:VAL:HG12	1.95	0.66
1:O:140:ILE:HD13	1:O:175:ARG:HD3	1.77	0.66
1:O:199:ASN:HD22	1:O:200:PRO:CD	2.07	0.66
1:P:37:PHE:HB2	1:P:77:LEU:HD12	1.76	0.66
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.11	0.66
1:E:184:MSE:HE3	1:E:191:LYS:CA	2.26	0.66
1:B:260:TYR:OH	1:B:271:ASP:HB3	1.96	0.66
1:E:241:LEU:CD2	1:E:241:LEU:N	2.56	0.66
1:J:184:MSE:CB	1:J:189:PRO:O	2.44	0.66
1:L:199:ASN:HD22	1:L:200:PRO:CD	2.08	0.66
1:M:176:ILE:CB	1:M:179:VAL:HG12	2.24	0.66
1:P:143:VAL:CG2	1:P:151:ILE:HD11	2.25	0.66
1:R:198:PRO:O	1:R:200:PRO:HD3	1.96	0.66
1:R:206:LEU:C	1:R:207:LEU:HD23	2.16	0.66
1:B:281:ARG:HG3	1:B:281:ARG:NH1	2.10	0.65
1:I:324:LEU:O	1:L:55:ARG:NH1	2.29	0.65
1:K:205:THR:CG2	1:K:207:LEU:H	2.09	0.65
1:L:23:LEU:O	1:L:26:PHE:HB2	1.95	0.65
1:M:175:ARG:HH11	1:M:177:PRO:HG3	1.58	0.65
1:O:126:PRO:HB2	1:O:127:PRO:HD3	1.77	0.65
1:A:125:TYR:CG	1:A:126:PRO:HD3	2.31	0.65
1:K:301:ASP:O	1:K:305:GLU:HB2	1.95	0.65
1:K:308:ASN:O	1:K:312:SER:HB2	1.96	0.65
1:P:254:GLU:N	1:P:254:GLU:CD	2.49	0.65
1:P:284:GLN:O	1:P:288:HIS:ND1	2.28	0.65
1:P:71:ASP:HB3	1:P:74:GLN:HB3	1.78	0.65
1:R:98:TYR:HB2	1:R:101:GLU:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:CD1	1:D:65:TYR:CZ	2.79	0.65
1:K:151:ILE:HA	1:K:154:THR:HG23	1.77	0.65
1:I:55:ARG:NH1	1:L:324:LEU:O	2.30	0.65
1:P:136:TYR:HB2	1:P:138:THR:HG22	1.79	0.65
1:B:60:ARG:HG2	1:B:287:TYR:OH	1.94	0.65
1:G:67:ALA:O	1:G:286:ARG:NH1	2.29	0.65
1:H:199:ASN:HD22	1:H:200:PRO:N	1.95	0.65
1:I:260:TYR:HA	1:I:263:LYS:HG2	1.79	0.65
1:I:288:HIS:O	1:I:292:GLU:HG2	1.95	0.65
1:P:64:LEU:HD21	1:P:207:LEU:HD21	1.78	0.65
1:N:99:ILE:HG12	1:Q:118:VAL:O	1.96	0.65
1:B:254:GLU:O	1:B:258:ARG:HG3	1.97	0.65
1:P:228:ILE:HG12	1:P:260:TYR:HB3	1.77	0.65
1:P:169:PHE:CE1	1:P:314:MSE:HE3	2.31	0.65
1:R:228:ILE:HG13	1:R:260:TYR:HB3	1.77	0.65
1:G:205:THR:HG22	1:G:207:LEU:N	2.08	0.65
1:M:324:LEU:O	1:P:55:ARG:NH1	2.30	0.65
1:R:279:THR:O	1:R:282:PRO:CD	2.43	0.65
1:G:101:GLU:CD	1:G:160:ARG:HH22	2.00	0.65
1:K:239:SER:O	1:K:242:LEU:HB2	1.96	0.65
1:L:313:GLU:HG3	1:L:317:LYS:HZ3	1.60	0.65
1:N:205:THR:CG2	1:N:207:LEU:H	2.08	0.65
1:B:199:ASN:HD22	1:B:201:LYS:H	1.45	0.65
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.80	0.65
1:E:57:ASN:OD1	1:E:60:ARG:NH1	2.30	0.65
1:G:252:SER:OG	1:G:255:GLU:HB2	1.96	0.65
1:P:254:GLU:O	1:P:257:GLU:N	2.30	0.65
1:C:188:ASP:HB3	1:C:191:LYS:HB2	1.78	0.65
1:E:210:ALA:HA	1:E:277:ILE:HG12	1.78	0.65
1:P:126:PRO:O	1:P:129:MSE:HB3	1.95	0.65
1:Q:67:ALA:O	1:Q:286:ARG:NH1	2.29	0.65
1:C:240:ASN:O	1:C:244:ILE:HG13	1.97	0.65
4:E:1003:AMP:H4'	4:E:1003:AMP:O3P	1.97	0.65
1:H:205:THR:CG2	1:H:207:LEU:H	2.03	0.65
1:L:23:LEU:HD13	1:L:65:TYR:CZ	2.33	0.65
1:O:199:ASN:ND2	1:O:200:PRO:HD2	2.12	0.65
1:B:8:ILE:HD13	1:B:65:TYR:CZ	2.32	0.64
1:D:18:ASN:ND2	4:D:1003:AMP:H5'1	2.12	0.64
1:E:67:ALA:O	1:E:286:ARG:NH1	2.30	0.64
1:I:260:TYR:HA	1:I:263:LYS:CG	2.27	0.64
1:J:72:PRO:HB3	1:J:299:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:THR:CB	1:K:149:GLN:HE22	2.09	0.64
1:I:99:ILE:HG13	1:L:118:VAL:HB	1.79	0.64
1:L:146:ASP:OD1	1:L:146:ASP:N	2.30	0.64
1:N:324:LEU:O	1:Q:55:ARG:NH1	2.31	0.64
1:R:50:ASP:HB3	1:R:53:GLU:HB2	1.79	0.64
1:A:199:ASN:HD22	1:A:200:PRO:HD2	1.62	0.64
1:B:252:SER:O	1:B:255:GLU:CB	2.46	0.64
1:B:67:ALA:O	1:B:286:ARG:NH1	2.30	0.64
1:E:245:TYR:O	1:E:249:SER:CB	2.44	0.64
1:F:43:HIS:HE1	1:F:132:ASP:OD2	1.78	0.64
1:M:187:VAL:HG22	1:M:202:ALA:HA	1.78	0.64
1:M:211:LYS:CD	1:Q:1:MSE:HG2	2.27	0.64
1:N:281:ARG:HB3	1:N:282:PRO:HD3	1.77	0.64
1:R:272:LEU:HD12	1:R:272:LEU:C	2.18	0.64
3:O:1002:PO4:O3	4:O:1003:AMP:H5'2	1.96	0.64
1:P:143:VAL:O	1:P:176:ILE:HD11	1.97	0.64
1:A:55:ARG:NH1	1:D:324:LEU:O	2.31	0.64
1:B:32:GLU:HG3	1:B:33:TYR:CD1	2.33	0.64
1:D:205:THR:CG2	1:D:207:LEU:H	2.10	0.64
1:A:55:ARG:NH2	1:D:320:GLN:NE2	2.46	0.64
1:D:56:GLN:O	1:D:60:ARG:HG3	1.97	0.64
4:E:1003:AMP:H5'2	4:E:1003:AMP:C8	2.33	0.64
1:E:238:ILE:CA	1:E:241:LEU:HD23	2.27	0.64
1:E:313:GLU:OE2	1:E:316:ARG:NH2	2.30	0.64
1:L:281:ARG:HG3	1:L:281:ARG:NH1	2.13	0.64
1:P:96:ILE:O	1:P:160:ARG:NH1	2.31	0.64
1:Q:176:ILE:HG12	1:Q:179:VAL:HB	1.79	0.64
1:Q:199:ASN:HD21	1:Q:201:LYS:HB2	1.63	0.64
1:P:228:ILE:HG23	1:P:238:ILE:CD1	2.28	0.64
1:P:71:ASP:HB3	1:P:74:GLN:CB	2.27	0.64
1:P:94:GLN:HA	1:P:97:VAL:HG12	1.80	0.64
1:I:19:TYR:CE2	1:I:24:ARG:HD3	2.33	0.64
1:I:281:ARG:HB3	1:I:282:PRO:HD3	1.80	0.64
1:K:22:ALA:O	1:K:26:PHE:CD2	2.51	0.64
1:N:278:GLU:OE1	1:N:281:ARG:NH2	2.30	0.64
1:O:146:ASP:N	1:O:146:ASP:OD1	2.29	0.64
1:O:162:ASN:HA	1:O:166:GLY:O	1.98	0.64
1:P:245:TYR:HE1	1:P:275:VAL:HG21	1.58	0.64
1:O:118:VAL:HG12	1:R:99:ILE:CD1	2.26	0.64
4:A:1003:AMP:H8	4:A:1003:AMP:C5'	2.11	0.64
1:E:184:MSE:CE	1:E:191:LYS:CA	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:GLU:OE2	1:G:298:ARG:NH1	2.30	0.64
1:J:134:LEU:HB3	1:J:169:PHE:CD1	2.32	0.64
1:N:145:GLU:HA	1:N:148:LYS:HG2	1.79	0.64
1:O:101:GLU:O	1:O:105:MSE:HE3	1.98	0.64
1:O:28:GLU:HA	1:O:31:HIS:HE1	1.62	0.64
1:O:313:GLU:OE2	1:O:316:ARG:NH1	2.28	0.64
1:Q:280:LEU:O	1:Q:284:GLN:HG3	1.98	0.64
1:B:24:ARG:HG2	1:B:24:ARG:O	1.96	0.64
1:E:84:PRO:O	1:E:88:GLN:HG3	1.97	0.64
1:G:5:PHE:HB2	1:G:138:THR:HG21	1.80	0.64
1:H:182:ARG:HG3	1:H:182:ARG:NH1	2.12	0.64
1:H:19:TYR:O	1:H:24:ARG:HB2	1.97	0.64
1:P:209:ASP:OD1	1:P:212:THR:CB	2.45	0.64
1:P:313:GLU:OE2	1:P:316:ARG:NH2	2.27	0.64
1:C:249:SER:OG	1:C:251:GLN:HG3	1.98	0.64
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.80	0.64
1:E:195:LYS:HG2	3:E:1002:PO4:O1	1.98	0.64
1:I:99:ILE:HG13	1:L:118:VAL:O	1.98	0.64
1:J:255:GLU:O	1:J:259:GLN:HB2	1.98	0.64
1:A:171:ILE:N	1:A:171:ILE:HD13	2.13	0.64
1:E:240:ASN:O	1:E:243:ASN:HB2	1.97	0.64
1:G:182:ARG:HG2	1:G:184:MSE:HE2	1.79	0.64
1:K:134:LEU:HB3	1:K:169:PHE:HD1	1.60	0.64
1:N:55:ARG:NH1	1:Q:324:LEU:O	2.29	0.64
1:Q:93:LEU:O	1:Q:97:VAL:HB	1.98	0.64
1:E:295:GLU:HG2	1:E:298:ARG:HH21	1.62	0.63
1:F:105:MSE:CA	1:F:105:MSE:HE2	2.27	0.63
1:P:195:LYS:NZ	3:P:1002:PO4:O1	2.30	0.63
3:P:1002:PO4:O3	4:P:1003:AMP:N7	2.31	0.63
1:Q:140:ILE:HD11	1:Q:175:ARG:HG3	0.73	0.63
1:E:237:GLY:O	1:E:241:LEU:HD21	1.97	0.63
1:F:99:ILE:O	1:F:103:GLU:HG3	1.98	0.63
1:G:280:LEU:O	1:G:284:GLN:HG3	1.96	0.63
1:L:141:VAL:HG12	1:L:143:VAL:HG13	1.79	0.63
1:O:67:ALA:O	1:O:286:ARG:NH1	2.30	0.63
1:P:215:LYS:O	1:P:215:LYS:HE2	1.97	0.63
1:P:245:TYR:CD1	1:P:272:LEU:HA	2.33	0.63
1:B:199:ASN:ND2	1:B:200:PRO:HD2	2.12	0.63
1:B:324:LEU:O	1:E:55:ARG:NH1	2.32	0.63
1:G:326:ARG:NH2	1:J:301:ASP:OD1	2.30	0.63
1:L:274:GLN:O	1:L:278:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:140:ILE:HD11	1:M:175:ARG:HD3	1.79	0.63
1:M:59:ARG:CZ	1:M:296:LEU:HD23	2.28	0.63
1:D:1:MSE:SE	1:O:211:LYS:HD2	2.49	0.63
1:A:209:ASP:O	1:A:213:ILE:HG13	1.97	0.63
1:D:99:ILE:O	1:D:103:GLU:HG3	1.97	0.63
1:F:105:MSE:HE2	1:F:105:MSE:HA	1.80	0.63
1:F:205:THR:HG22	1:F:207:LEU:N	2.13	0.63
1:G:118:VAL:HB	1:J:99:ILE:HG13	1.79	0.63
1:K:22:ALA:O	1:K:26:PHE:CE2	2.50	0.63
1:I:55:ARG:HH22	1:L:320:GLN:NE2	1.93	0.63
1:O:205:THR:HG22	1:O:207:LEU:N	2.11	0.63
1:P:195:LYS:H	3:P:1002:PO4:P	2.21	0.63
1:R:274:GLN:HA	1:R:277:ILE:HD12	1.79	0.63
1:E:71:ASP:OD1	1:E:73:THR:HG23	1.99	0.63
1:R:218:LYS:HG2	1:R:219:SER:H	1.63	0.63
1:B:2:LYS:N	1:B:2:LYS:HD2	2.13	0.63
1:C:193:MSE:HB3	4:C:1003:AMP:N6	2.14	0.63
1:C:324:LEU:O	1:F:55:ARG:NH1	2.31	0.63
1:E:107:GLN:CD	1:E:150:HIS:HE2	2.02	0.63
1:N:245:TYR:HD1	1:N:272:LEU:CD1	2.12	0.63
1:E:245:TYR:HA	1:E:272:LEU:HD13	1.78	0.63
1:B:320:GLN:HE22	1:E:55:ARG:NH2	1.96	0.63
1:K:16:ILE:HD13	1:K:204:ILE:HB	1.79	0.63
1:M:184:MSE:SE	1:M:191:LYS:O	2.67	0.63
1:P:245:TYR:HD1	1:P:272:LEU:CD1	2.12	0.63
1:D:214:GLU:O	1:D:218:LYS:HG3	1.98	0.63
1:E:217:ILE:HD12	1:E:273:ALA:HA	1.80	0.63
1:H:56:GLN:O	1:H:60:ARG:HG3	1.99	0.63
1:P:271:ASP:O	1:P:275:VAL:CG2	2.35	0.63
1:B:246:SER:HB2	1:B:251:GLN:O	1.99	0.63
1:K:238:ILE:HA	1:K:241:LEU:CD1	2.28	0.63
1:K:256:LEU:CD2	1:K:259:GLN:HG2	2.29	0.63
1:H:324:LEU:O	1:K:55:ARG:NH1	2.32	0.63
1:L:41:ASP:OD2	1:L:81:SER:HB3	1.98	0.63
1:O:324:LEU:O	1:R:55:ARG:NH1	2.32	0.63
1:D:182:ARG:HE	1:D:192:LYS:HG3	1.64	0.62
1:E:101:GLU:O	1:E:105:MSE:HE3	1.99	0.62
1:E:267:VAL:HG13	1:E:268:PHE:H	1.63	0.62
1:E:276:VAL:O	1:E:280:LEU:HG	1.99	0.62
1:H:55:ARG:NH1	1:K:324:LEU:O	2.32	0.62
1:M:165:TYR:CE1	1:M:322:MSE:HG2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ILE:HB	1:M:82:GLU:HG3	1.81	0.62
1:P:15:THR:HG22	1:P:203:TYR:HB2	1.80	0.62
1:A:18:ASN:HD21	4:A:1003:AMP:C5'	2.04	0.62
1:G:302:GLU:O	1:G:306:LYS:HG3	1.99	0.62
1:O:25:GLN:HG3	1:O:29:LEU:HD11	1.80	0.62
1:E:106:THR:HB	1:E:149:GLN:OE1	1.98	0.62
1:G:129:MSE:HE3	2:G:1001:TRP:CE3	2.34	0.62
1:G:313:GLU:OE2	1:G:316:ARG:NH2	2.33	0.62
1:H:133:ILE:O	1:H:138:THR:HG23	1.99	0.62
1:O:19:TYR:CE2	1:O:24:ARG:HD3	2.34	0.62
1:P:126:PRO:CD	1:P:127:PRO:HD2	2.27	0.62
1:E:3:THR:HB	1:E:138:THR:HA	1.81	0.62
1:I:19:TYR:O	1:I:24:ARG:CB	2.46	0.62
1:K:122:LEU:O	1:K:125:TYR:HE1	1.83	0.62
1:M:147:GLN:O	1:M:151:ILE:HG12	2.00	0.62
1:Q:200:PRO:HA	1:Q:203:TYR:CE2	2.34	0.62
1:D:142:PRO:HA	1:D:175:ARG:O	1.99	0.62
1:E:240:ASN:O	1:E:244:ILE:HG13	2.00	0.62
1:F:71:ASP:OD1	1:F:73:THR:HG23	2.00	0.62
1:K:238:ILE:CA	1:K:241:LEU:HD11	2.30	0.62
4:M:1003:AMP:C3'	4:M:1003:AMP:O1P	2.46	0.62
1:N:265:TYR:O	1:N:269:LYS:HG3	1.99	0.62
1:P:205:THR:CG2	1:P:207:LEU:H	2.13	0.62
1:Q:107:GLN:H	1:Q:107:GLN:CD	2.01	0.62
1:K:126:PRO:N	1:K:127:PRO:CD	2.63	0.62
1:P:245:TYR:CD2	1:P:256:LEU:CD1	2.81	0.62
1:B:200:PRO:HA	1:B:203:TYR:CE2	2.35	0.62
1:G:193:MSE:O	4:G:1003:AMP:N6	2.32	0.62
1:I:5:PHE:HB2	1:I:138:THR:HG21	1.79	0.62
1:J:254:GLU:OE1	1:J:254:GLU:N	2.32	0.62
1:K:134:LEU:CB	1:K:169:PHE:CE1	2.80	0.62
1:R:228:ILE:CG2	1:R:260:TYR:HB3	2.25	0.62
1:A:102:LEU:O	1:A:105:MSE:HB2	1.99	0.62
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.35	0.62
1:E:253:ILE:O	1:E:257:GLU:HB2	2.00	0.62
1:M:271:ASP:OD1	1:Q:309:ARG:NE	2.32	0.62
1:N:272:LEU:O	1:N:276:VAL:HG23	2.00	0.62
1:N:288:HIS:O	1:N:292:GLU:HG2	2.00	0.62
1:Q:182:ARG:HE	1:Q:184:MSE:HE1	1.64	0.62
1:R:106:THR:H	1:R:149:GLN:HE22	1.48	0.62
1:R:19:TYR:CE2	1:R:24:ARG:CG	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:VAL:HG12	1:E:180:GLY:O	2.00	0.62
1:J:187:VAL:HG22	1:J:202:ALA:CB	2.29	0.62
1:J:86:HIS:HD2	1:J:132:ASP:OD1	1.82	0.62
1:N:205:THR:HG22	1:N:207:LEU:N	2.09	0.62
1:O:105:MSE:CA	1:O:105:MSE:HE2	2.28	0.62
1:O:30:GLN:OE1	1:O:71:ASP:N	2.31	0.62
1:P:206:LEU:N	1:P:206:LEU:HD23	2.14	0.62
1:R:185:SER:HB3	1:R:188:ASP:O	1.98	0.62
1:B:254:GLU:OE1	1:B:254:GLU:N	2.32	0.62
1:C:309:ARG:NH1	1:D:271:ASP:OD1	2.33	0.62
1:J:193:MSE:HB3	4:J:1003:AMP:N6	2.15	0.62
1:M:240:ASN:O	1:M:244:ILE:HG13	2.00	0.62
1:M:280:LEU:O	1:M:284:GLN:CG	2.45	0.62
1:P:118:VAL:CG1	1:P:122:LEU:CD1	2.78	0.62
1:P:213:ILE:HG22	1:P:217:ILE:HD12	1.82	0.62
1:B:205:THR:HG22	1:B:208:ASP:N	2.14	0.61
1:K:106:THR:OG1	1:K:149:GLN:NE2	2.33	0.61
1:K:185:SER:HB3	1:K:188:ASP:O	1.99	0.61
1:O:253:ILE:HG22	1:O:257:GLU:OE2	2.00	0.61
1:O:280:LEU:HB3	1:O:284:GLN:OE1	2.00	0.61
1:P:126:PRO:HD2	1:P:127:PRO:CD	2.30	0.61
1:P:16:ILE:CD1	1:P:193:MSE:HE1	2.26	0.61
1:P:308:ASN:O	1:P:312:SER:HB2	1.99	0.61
1:R:106:THR:H	1:R:149:GLN:NE2	1.98	0.61
1:R:29:LEU:CD1	1:R:177:PRO:HG2	2.29	0.61
1:A:274:GLN:O	1:A:278:GLU:HG2	2.00	0.61
1:K:176:ILE:O	1:K:179:VAL:HG22	2.01	0.61
1:P:25:GLN:HG2	1:P:178:LYS:HB3	1.81	0.61
1:C:29:LEU:HD22	1:C:33:TYR:CD1	2.35	0.61
1:F:280:LEU:O	1:F:284:GLN:HG3	2.01	0.61
1:P:193:MSE:HB3	4:P:1003:AMP:HN61	1.64	0.61
1:P:251:GLN:HG3	1:P:256:LEU:HD11	1.82	0.61
1:P:245:TYR:HD1	1:P:272:LEU:HA	1.65	0.61
1:P:319:GLU:HB3	1:P:324:LEU:HB2	1.80	0.61
1:B:29:LEU:HD22	1:B:33:TYR:HE1	1.65	0.61
1:M:55:ARG:HD2	1:P:325:GLY:O	2.01	0.61
1:P:266:GLY:O	1:P:270:ALA:HB2	2.00	0.61
1:R:162:ASN:HA	1:R:166:GLY:O	2.00	0.61
1:P:253:ILE:CG2	1:P:254:GLU:CD	2.59	0.61
1:R:133:ILE:O	1:R:138:THR:CG2	2.45	0.61
1:F:228:ILE:O	1:F:229:ARG:CG	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:LEU:HB3	1:J:268:PHE:HE2	1.64	0.61
1:M:133:ILE:O	1:M:138:THR:HG23	2.00	0.61
1:P:175:ARG:HG2	1:P:176:ILE:N	2.14	0.61
1:R:284:GLN:O	1:R:288:HIS:ND1	2.31	0.61
1:B:214:GLU:O	1:B:218:LYS:HG3	2.01	0.61
1:B:253:ILE:HG22	1:B:257:GLU:OE1	2.01	0.61
1:G:212:THR:CG2	1:G:216:LYS:HE3	2.31	0.61
1:M:305:GLU:O	1:M:309:ARG:HG3	2.01	0.61
1:O:31:HIS:N	1:O:31:HIS:ND1	2.48	0.61
1:P:60:ARG:HD2	1:P:287:TYR:OH	2.00	0.61
1:R:19:TYR:O	1:R:24:ARG:HG3	2.00	0.61
1:E:267:VAL:HG13	1:E:268:PHE:N	2.15	0.61
1:L:60:ARG:HG2	1:L:287:TYR:OH	2.00	0.61
1:O:185:SER:HB2	1:O:202:ALA:HB1	1.83	0.61
1:P:176:ILE:CB	1:P:179:VAL:HG22	2.26	0.61
1:C:306:LYS:HA	1:D:267:VAL:HG12	1.82	0.61
3:F:1002:PO4:O1	4:F:1003:AMP:H5'2	2.01	0.61
1:H:86:HIS:HD2	1:H:132:ASP:OD1	1.83	0.61
1:M:297:ASP:OD2	1:P:326:ARG:NH1	2.33	0.61
1:P:161:PHE:C	1:P:161:PHE:CD2	2.73	0.61
1:B:260:TYR:OH	1:B:271:ASP:CG	2.39	0.60
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.82	0.60
1:E:19:TYR:HE1	1:E:68:VAL:CG1	2.13	0.60
1:H:249:SER:OG	1:H:251:GLN:HG3	2.01	0.60
1:J:213:ILE:O	1:J:217:ILE:HG13	2.00	0.60
1:P:118:VAL:HG12	1:P:122:LEU:HD12	1.83	0.60
1:J:205:THR:HG22	1:J:207:LEU:N	2.14	0.60
1:K:125:TYR:CG	1:K:126:PRO:HD3	2.36	0.60
1:O:65:TYR:O	1:O:70:ILE:HB	2.01	0.60
1:E:284:GLN:O	1:E:288:HIS:HD2	1.83	0.60
1:F:205:THR:HG23	1:F:207:LEU:H	1.65	0.60
1:I:245:TYR:O	1:I:245:TYR:HD1	1.83	0.60
1:O:183:ILE:O	4:O:1003:AMP:N6	2.27	0.60
1:R:184:MSE:HE3	1:R:192:LYS:HA	1.82	0.60
1:C:67:ALA:O	1:C:286:ARG:NH1	2.34	0.60
1:D:278:GLU:OE2	1:D:281:ARG:NH2	2.35	0.60
1:G:224:SER:HB2	1:I:166:GLY:N	2.16	0.60
1:K:208:ASP:O	1:K:284:GLN:NE2	2.34	0.60
1:L:105:MSE:HE2	1:L:150:HIS:CE1	2.35	0.60
1:M:120:ALA:HB2	1:P:102:LEU:CD1	2.30	0.60
1:M:241:LEU:HB3	1:M:268:PHE:CE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HB3	1:B:282:PRO:CD	2.32	0.60
1:D:308:ASN:O	1:D:312:SER:HB2	2.01	0.60
1:G:55:ARG:NH1	1:J:324:LEU:O	2.34	0.60
1:R:218:LYS:CG	1:R:219:SER:N	2.63	0.60
1:I:147:GLN:O	1:I:151:ILE:HG12	2.01	0.60
1:R:43:HIS:HE1	1:R:132:ASP:OD2	1.84	0.60
1:R:27:VAL:HG23	1:R:28:GLU:HG2	1.83	0.60
1:B:4:ILE:HG12	1:B:140:ILE:HB	1.82	0.60
1:E:184:MSE:CE	1:E:191:LYS:N	2.64	0.60
1:F:19:TYR:CZ	1:F:24:ARG:HG3	2.37	0.60
1:K:228:ILE:HG22	1:K:228:ILE:O	2.02	0.60
1:M:229:ARG:HG3	1:M:257:GLU:HG2	1.83	0.60
1:O:26:PHE:CD2	1:O:29:LEU:CD1	2.82	0.60
1:B:125:TYR:N	1:B:126:PRO:CD	2.65	0.60
1:H:43:HIS:HE1	1:H:132:ASP:OD2	1.84	0.60
1:P:244:ILE:HG22	1:P:272:LEU:HD11	1.84	0.60
1:R:147:GLN:HA	1:R:150:HIS:HD2	1.65	0.60
1:A:84:PRO:HD2	1:A:308:ASN:HD21	1.67	0.60
1:B:100:GLY:O	1:B:104:ARG:HG2	2.02	0.60
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.85	0.60
1:G:99:ILE:HG13	1:J:118:VAL:HB	1.83	0.60
1:K:185:SER:N	1:K:191:LYS:O	2.33	0.60
1:P:118:VAL:CG1	1:P:122:LEU:HD12	2.32	0.60
1:Q:125:TYR:CD2	1:Q:126:PRO:HD3	2.36	0.60
1:A:151:ILE:HG21	1:A:174:ALA:HB2	1.83	0.60
1:B:255:GLU:CA	1:B:258:ARG:HH21	2.14	0.60
1:E:253:ILE:CG1	1:E:253:ILE:O	2.49	0.60
1:E:315:VAL:O	1:E:319:GLU:HG3	2.02	0.60
1:G:105:MSE:HE2	1:G:105:MSE:HA	1.83	0.60
1:G:313:GLU:HG3	1:G:317:LYS:HZ3	1.66	0.60
1:K:86:HIS:HD2	1:K:132:ASP:OD1	1.85	0.60
4:P:1003:AMP:H2'	4:P:1003:AMP:N3	2.16	0.60
1:P:124:THR:CA	1:P:126:PRO:HD2	2.32	0.60
1:E:29:LEU:HD11	1:E:177:PRO:HB2	1.83	0.59
1:E:71:ASP:HB3	1:E:74:GLN:HB2	1.84	0.59
1:G:193:MSE:HE2	1:G:203:TYR:HA	1.83	0.59
1:H:22:ALA:O	1:H:26:PHE:CE2	2.54	0.59
1:I:16:ILE:HG12	1:I:204:ILE:HB	1.83	0.59
1:A:124:THR:HG21	1:D:94:GLN:HE21	1.67	0.59
1:C:316:ARG:CG	1:C:316:ARG:HH21	2.13	0.59
1:K:287:TYR:CZ	1:K:291:MSE:CE	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:282:PRO:O	1:L:286:ARG:HG3	2.02	0.59
1:M:64:LEU:HD23	1:M:287:TYR:HD1	1.64	0.59
1:P:245:TYR:CD1	1:P:272:LEU:HD12	2.36	0.59
1:Q:29:LEU:HD11	1:Q:177:PRO:HB2	1.84	0.59
1:A:184:MSE:HB3	1:A:191:LYS:O	2.03	0.59
1:J:155:ARG:HG2	1:J:171:ILE:HG23	1.83	0.59
1:K:245:TYR:HE1	1:K:275:VAL:CG1	2.13	0.59
1:L:23:LEU:CD1	1:L:65:TYR:CE2	2.85	0.59
1:N:126:PRO:CB	1:N:127:PRO:HD3	2.29	0.59
1:Q:199:ASN:ND2	1:Q:201:LYS:H	1.99	0.59
1:R:105:MSE:HA	1:R:149:GLN:OE1	2.02	0.59
1:E:197:ASP:OD1	1:E:198:PRO:HD2	2.03	0.59
4:I:1003:AMP:C8	4:I:1003:AMP:H5'1	2.37	0.59
1:I:90:ALA:O	1:I:94:GLN:HG3	2.01	0.59
1:J:39:ILE:HG23	1:J:61:LEU:HD23	1.83	0.59
1:H:48:TRP:CZ2	1:K:164:ARG:NH1	2.70	0.59
1:K:314:MSE:O	1:K:318:MSE:HG3	2.02	0.59
1:L:171:ILE:O	1:L:171:ILE:HG22	2.02	0.59
1:P:254:GLU:O	1:P:258:ARG:N	2.30	0.59
1:M:164:ARG:NH1	1:P:48:TRP:CZ2	2.69	0.59
1:A:318:MSE:O	1:A:322:MSE:HG3	2.02	0.59
1:D:18:ASN:HD21	4:D:1003:AMP:H5'1	1.67	0.59
1:H:134:LEU:HB3	1:H:169:PHE:CE1	2.38	0.59
1:I:3:THR:HB	1:I:138:THR:HA	1.83	0.59
1:N:56:GLN:OE1	1:N:60:ARG:NH2	2.35	0.59
1:R:253:ILE:O	1:R:257:GLU:CB	2.50	0.59
1:O:326:ARG:NH1	1:R:300:LEU:HB2	2.17	0.59
1:B:38:CYS:SG	1:B:80:GLN:HB2	2.42	0.59
1:F:278:GLU:OE1	1:F:278:GLU:HA	2.03	0.59
1:G:193:MSE:HB3	4:G:1003:AMP:N6	2.18	0.59
1:H:206:LEU:HD23	1:H:206:LEU:N	2.17	0.59
1:I:26:PHE:O	1:I:30:GLN:HG2	2.02	0.59
1:J:125:TYR:N	1:J:126:PRO:CD	2.65	0.59
1:J:295:GLU:OE2	1:J:298:ARG:NH2	2.27	0.59
1:M:146:ASP:OD1	1:M:146:ASP:N	2.30	0.59
1:O:18:ASN:HA	4:O:1003:AMP:C1'	2.30	0.59
1:E:125:TYR:N	1:E:126:PRO:HD2	2.17	0.59
1:E:26:PHE:CD1	1:E:37:PHE:HE2	2.20	0.59
1:K:259:GLN:O	1:K:263:LYS:HE2	2.02	0.59
1:N:213:ILE:HD11	1:N:280:LEU:HD12	1.84	0.59
1:A:133:ILE:O	1:A:138:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:142:PRO:HA	1:N:175:ARG:O	2.03	0.59
1:P:267:VAL:HG23	1:P:268:PHE:N	2.17	0.59
1:R:272:LEU:O	1:R:275:VAL:HG13	2.02	0.59
1:B:313:GLU:OE2	1:B:316:ARG:NH2	2.32	0.59
1:E:30:GLN:CG	1:E:74:GLN:HG2	2.31	0.59
1:K:59:ARG:NH2	1:K:296:LEU:HD23	2.17	0.59
1:N:295:GLU:OE2	1:N:298:ARG:NH2	2.32	0.59
1:Q:185:SER:O	1:Q:188:ASP:O	2.20	0.59
1:Q:199:ASN:ND2	1:Q:201:LYS:HB2	2.18	0.59
1:R:187:VAL:HG13	1:R:201:LYS:HB2	1.85	0.59
1:R:291:MSE:HE3	1:R:291:MSE:CA	2.32	0.59
1:E:245:TYR:HA	1:E:272:LEU:CD1	2.33	0.59
1:F:83:VAL:HG13	1:F:308:ASN:HA	1.83	0.59
1:H:125:TYR:N	1:H:126:PRO:CD	2.66	0.59
1:M:105:MSE:HE2	1:M:150:HIS:ND1	2.09	0.59
1:M:253:ILE:O	1:M:257:GLU:HB2	2.03	0.59
4:B:1003:AMP:H8	4:B:1003:AMP:H5'1	1.66	0.58
1:E:52:HIS:O	1:E:56:GLN:HB2	2.02	0.58
1:G:125:TYR:N	1:G:126:PRO:CD	2.66	0.58
1:K:238:ILE:C	1:K:241:LEU:CD1	2.71	0.58
1:M:209:ASP:OD1	1:M:212:THR:CB	2.50	0.58
1:M:42:GLN:HB2	1:M:80:GLN:OE1	2.03	0.58
1:Q:38:CYS:SG	1:Q:80:GLN:HB2	2.43	0.58
1:A:105:MSE:CE	1:A:105:MSE:HA	2.32	0.58
1:J:129:MSE:HE3	2:J:1001:TRP:CE3	2.38	0.58
1:J:217:ILE:O	1:J:269:LYS:HD3	2.03	0.58
1:M:99:ILE:O	1:M:103:GLU:HG3	2.03	0.58
1:N:203:TYR:O	1:N:216:LYS:NZ	2.33	0.58
1:Q:19:TYR:CE2	1:Q:24:ARG:HD3	2.38	0.58
1:B:241:LEU:HB3	1:B:268:PHE:HE2	1.68	0.58
1:C:41:ASP:OD2	1:C:81:SER:HB3	2.03	0.58
1:D:240:ASN:O	1:D:244:ILE:HG13	2.03	0.58
1:G:105:MSE:CA	1:G:105:MSE:HE2	2.33	0.58
1:H:141:VAL:HG12	1:H:143:VAL:HG13	1.83	0.58
1:I:281:ARG:HB3	1:I:282:PRO:CD	2.33	0.58
1:J:101:GLU:O	1:J:105:MSE:HE2	2.00	0.58
1:K:183:ILE:N	1:K:183:ILE:HD13	2.17	0.58
1:O:281:ARG:N	1:O:282:PRO:HD2	2.18	0.58
1:Q:272:LEU:HA	1:Q:275:VAL:HG13	1.83	0.58
1:R:199:ASN:OD1	1:R:201:LYS:CB	2.51	0.58
1:B:55:ARG:NH1	1:E:324:LEU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ALA:O	1:F:26:PHE:CE2	2.55	0.58
1:I:86:HIS:HD2	1:I:132:ASP:OD1	1.87	0.58
1:J:60:ARG:HG2	1:J:287:TYR:OH	2.03	0.58
1:M:16:ILE:O	1:M:20:ILE:HG13	2.03	0.58
1:N:90:ALA:O	1:N:94:GLN:HG3	2.03	0.58
1:R:125:TYR:N	1:R:126:PRO:CD	2.67	0.58
1:C:215:LYS:O	1:C:219:SER:OG	2.20	0.58
1:G:126:PRO:CB	1:G:127:PRO:HD3	2.33	0.58
1:H:126:PRO:HB2	1:H:127:PRO:CD	2.33	0.58
1:I:199:ASN:ND2	1:I:200:PRO:CD	2.31	0.58
1:O:89:ALA:HB2	1:O:135:LEU:HD21	1.84	0.58
1:P:118:VAL:HG12	1:P:122:LEU:HD11	1.85	0.58
1:A:105:MSE:HE2	1:A:105:MSE:N	2.17	0.58
1:I:313:GLU:OE2	1:I:316:ARG:NH2	2.30	0.58
1:K:205:THR:HG22	1:K:207:LEU:N	2.16	0.58
1:P:241:LEU:HB3	1:P:272:LEU:HD22	1.86	0.58
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.86	0.58
1:C:129:MSE:HE3	2:C:1001:TRP:CE3	2.39	0.58
1:D:31:HIS:O	1:O:215:LYS:HE2	2.03	0.58
1:B:118:VAL:CG1	1:E:99:ILE:HD12	2.34	0.58
1:O:56:GLN:O	1:O:60:ARG:HB2	2.04	0.58
1:P:126:PRO:CG	1:P:127:PRO:CD	2.76	0.58
1:P:71:ASP:O	1:P:75:ALA:N	2.36	0.58
1:R:16:ILE:O	1:R:20:ILE:CG1	2.49	0.58
1:B:295:GLU:O	1:B:299:VAL:HG23	2.03	0.58
1:F:23:LEU:CD2	1:F:68:VAL:HG11	2.33	0.58
1:G:320:GLN:NE2	1:J:55:ARG:NH2	2.52	0.58
1:M:200:PRO:O	1:M:216:LYS:NZ	2.32	0.58
1:M:281:ARG:N	1:M:282:PRO:HD2	2.18	0.58
1:M:56:GLN:NE2	1:M:60:ARG:NH2	2.52	0.58
1:O:142:PRO:HA	1:O:175:ARG:O	2.04	0.58
1:B:319:GLU:O	1:B:323:GLY:N	2.32	0.58
1:D:147:GLN:O	1:D:151:ILE:HG12	2.03	0.58
1:H:199:ASN:HD21	1:H:201:LYS:HB2	1.68	0.58
1:J:168:LEU:HD11	1:J:317:LYS:HD3	1.85	0.58
1:O:273:ALA:O	1:O:277:ILE:HG13	2.03	0.58
1:O:72:PRO:HB3	1:O:299:VAL:HG13	1.85	0.58
1:P:245:TYR:CD1	1:P:272:LEU:CD1	2.86	0.58
1:Q:157:LEU:CD2	1:Q:160:ARG:HH21	2.17	0.58
1:Q:190:THR:HG23	1:Q:190:THR:O	2.03	0.58
1:A:315:VAL:O	1:A:319:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.39	0.57
1:D:175:ARG:O	1:D:177:PRO:HD3	2.04	0.57
1:H:277:ILE:O	1:H:281:ARG:HB2	2.04	0.57
1:H:59:ARG:NH2	1:H:297:ASP:OD1	2.27	0.57
1:H:5:PHE:HB2	1:H:138:THR:HG21	1.86	0.57
1:M:64:LEU:HD21	1:M:287:TYR:CD1	2.36	0.57
1:Q:24:ARG:HH11	1:Q:24:ARG:CG	2.17	0.57
1:Q:281:ARG:NH1	1:Q:281:ARG:HG3	2.14	0.57
1:O:297:ASP:OD2	1:R:326:ARG:NH1	2.37	0.57
1:B:205:THR:HG22	1:B:207:LEU:H	1.69	0.57
1:E:96:ILE:O	1:E:160:ARG:NH1	2.37	0.57
1:E:176:ILE:HB	1:E:179:VAL:HG22	1.85	0.57
1:F:200:PRO:O	1:F:216:LYS:NZ	2.37	0.57
1:K:124:THR:O	1:K:127:PRO:CG	2.52	0.57
1:M:295:GLU:HG3	1:M:295:GLU:O	2.04	0.57
1:O:254:GLU:O	1:O:258:ARG:HB2	2.04	0.57
1:P:16:ILE:HD13	1:P:204:ILE:HB	1.86	0.57
1:Q:272:LEU:O	1:Q:276:VAL:HG23	2.04	0.57
1:R:281:ARG:N	1:R:282:PRO:HD2	2.18	0.57
1:B:72:PRO:O	1:B:306:LYS:NZ	2.33	0.57
1:C:141:VAL:HG12	1:C:143:VAL:HG13	1.86	0.57
1:E:99:ILE:O	1:E:103:GLU:HG3	2.04	0.57
1:H:241:LEU:HB3	1:H:268:PHE:HE2	1.69	0.57
1:K:124:THR:C	1:K:127:PRO:HD2	2.24	0.57
1:O:175:ARG:HH22	1:O:177:PRO:HB3	1.66	0.57
1:P:9:GLN:HE21	1:P:9:GLN:HA	1.68	0.57
1:R:141:VAL:HG12	1:R:143:VAL:HG13	1.86	0.57
1:C:126:PRO:HB2	1:C:127:PRO:CD	2.33	0.57
1:D:278:GLU:HA	1:D:278:GLU:OE1	2.04	0.57
1:L:165:TYR:HB3	1:L:321:ALA:HB1	1.85	0.57
1:O:84:PRO:O	1:O:88:GLN:HG3	2.03	0.57
1:R:282:PRO:O	1:R:286:ARG:CG	2.50	0.57
1:A:193:MSE:HB3	4:A:1003:AMP:N6	2.20	0.57
1:B:199:ASN:ND2	1:B:201:LYS:H	2.03	0.57
1:B:245:TYR:CD2	1:B:272:LEU:HB2	2.40	0.57
1:H:260:TYR:CD1	1:H:263:LYS:HG3	2.39	0.57
1:J:185:SER:O	1:J:189:PRO:HA	2.04	0.57
1:J:79:ILE:HB	1:J:82:GLU:HG3	1.87	0.57
1:M:98:TYR:N	1:M:101:GLU:OE1	2.22	0.57
1:M:22:ALA:O	1:M:26:PHE:CD2	2.57	0.57
1:O:254:GLU:CD	1:O:254:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:145:GLU:N	1:P:145:GLU:OE1	2.33	0.57
4:Q:1003:AMP:H8	4:Q:1003:AMP:C5'	2.17	0.57
1:H:30:GLN:O	1:H:74:GLN:NE2	2.38	0.57
1:I:38:CYS:SG	1:I:80:GLN:HB2	2.45	0.57
1:L:8:ILE:HD13	1:L:65:TYR:OH	2.04	0.57
1:P:246:SER:HA	1:P:249:SER:HG	1.68	0.57
1:P:241:LEU:HD22	1:P:272:LEU:HD21	1.86	0.57
1:A:146:ASP:N	1:A:146:ASP:OD1	2.37	0.57
1:C:19:TYR:HB2	1:C:206:LEU:HD21	1.86	0.57
1:C:56:GLN:O	1:C:60:ARG:HG3	2.05	0.57
1:E:240:ASN:HB3	1:E:241:LEU:HD22	1.87	0.57
1:P:106:THR:O	1:P:106:THR:HG22	2.04	0.57
1:R:203:TYR:O	1:R:216:LYS:HD3	2.04	0.57
1:R:291:MSE:HA	1:R:291:MSE:HE3	1.86	0.57
3:F:1002:PO4:O1	4:F:1003:AMP:H8	1.87	0.57
1:G:136:TYR:HB2	1:G:138:THR:HG22	1.87	0.57
1:G:146:ASP:N	1:G:146:ASP:OD1	2.29	0.57
1:H:230:TYR:C	1:H:230:TYR:CD1	2.78	0.57
1:K:258:ARG:HA	1:K:261:GLU:HG3	1.86	0.57
1:L:125:TYR:N	1:L:126:PRO:CD	2.68	0.57
1:O:325:GLY:C	1:O:326:ARG:HG3	2.24	0.57
1:P:20:ILE:CD1	1:P:183:ILE:CD1	2.74	0.57
1:Q:133:ILE:O	1:Q:138:THR:CG2	2.53	0.57
1:C:214:GLU:O	1:C:218:LYS:HG3	2.04	0.57
1:E:146:ASP:N	1:E:146:ASP:OD1	2.36	0.57
1:K:7:GLY:C	1:K:8:ILE:HD13	2.25	0.57
1:L:133:ILE:O	1:L:138:THR:HG23	2.04	0.57
1:I:326:ARG:NH1	1:L:297:ASP:OD2	2.35	0.57
1:M:311:ALA:O	1:M:314:MSE:N	2.38	0.57
1:M:8:ILE:HD12	1:M:65:TYR:CZ	2.40	0.57
1:P:247:THR:OG1	1:P:248:LEU:CD1	2.51	0.57
1:R:184:MSE:HE3	1:R:192:LYS:CA	2.35	0.57
1:R:19:TYR:CE2	1:R:24:ARG:HG2	2.40	0.57
1:E:197:ASP:HB3	1:E:202:ALA:HB3	1.86	0.57
1:L:313:GLU:OE2	1:L:317:LYS:NZ	2.37	0.57
1:B:255:GLU:HA	1:B:258:ARG:NH2	2.20	0.56
1:M:118:VAL:HB	1:P:99:ILE:HG13	1.87	0.56
1:N:55:ARG:NH2	1:Q:320:GLN:HE21	2.03	0.56
1:R:136:TYR:HB2	1:R:138:THR:HG22	1.86	0.56
1:D:96:ILE:HD12	1:D:160:ARG:HG2	1.86	0.56
1:J:256:LEU:O	1:J:260:TYR:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ILE:HG22	1:L:61:LEU:HD21	1.86	0.56
1:Q:212:THR:HG22	1:Q:216:LYS:HE3	1.86	0.56
1:A:18:ASN:ND2	4:A:1003:AMP:C8	2.73	0.56
1:A:168:LEU:O	1:A:314:MSE:HE1	2.06	0.56
1:A:71:ASP:HB3	1:A:74:GLN:HB2	1.87	0.56
1:B:315:VAL:O	1:B:319:GLU:HG3	2.05	0.56
1:B:94:GLN:NE2	1:E:124:THR:CB	2.68	0.56
1:N:176:ILE:HB	1:N:179:VAL:HG13	1.86	0.56
1:P:16:ILE:HG12	1:P:17:GLY:H	1.69	0.56
1:Q:139:ASP:OD1	1:Q:170:THR:HG21	2.04	0.56
1:F:184:MSE:HE2	1:F:189:PRO:O	2.05	0.56
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.88	0.56
1:P:3:THR:HB	1:P:138:THR:HA	1.87	0.56
1:R:171:ILE:N	1:R:171:ILE:HD13	2.19	0.56
1:R:91:TRP:HE3	1:R:94:GLN:OE1	1.88	0.56
1:R:94:GLN:HA	1:R:97:VAL:HG12	1.87	0.56
1:B:230:TYR:CD1	1:B:239:SER:HB3	2.41	0.56
1:B:286:ARG:HA	1:B:289:HIS:HB3	1.87	0.56
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.41	0.56
1:O:24:ARG:CG	1:O:24:ARG:HH11	2.19	0.56
1:P:248:LEU:CD1	1:P:248:LEU:N	2.67	0.56
1:R:19:TYR:CE2	1:R:24:ARG:CD	2.88	0.56
1:E:243:ASN:O	1:E:247:THR:CG2	2.53	0.56
1:L:86:HIS:HD2	1:L:132:ASP:OD1	1.88	0.56
1:P:195:LYS:N	3:P:1002:PO4:O2	2.37	0.56
1:B:29:LEU:HD22	1:B:33:TYR:CE1	2.40	0.56
1:C:38:CYS:SG	1:C:80:GLN:HB2	2.46	0.56
1:H:145:GLU:O	1:H:148:LYS:HG2	2.05	0.56
1:I:273:ALA:O	1:I:277:ILE:HD12	2.05	0.56
1:N:125:TYR:N	1:N:126:PRO:CD	2.69	0.56
1:P:245:TYR:HE1	1:P:275:VAL:CG2	2.17	0.56
1:Q:59:ARG:NH2	1:Q:296:LEU:HD23	2.20	0.56
1:Q:79:ILE:HB	1:Q:82:GLU:HG3	1.86	0.56
1:R:195:LYS:HG2	3:R:1002:PO4:O1	2.05	0.56
1:R:29:LEU:HD11	1:R:177:PRO:HG2	1.87	0.56
1:H:293:SER:OG	1:H:295:GLU:HB2	2.05	0.56
1:K:147:GLN:OE1	1:K:150:HIS:HD2	1.89	0.56
1:Q:151:ILE:HG13	1:Q:174:ALA:HB2	1.88	0.56
1:R:126:PRO:CB	1:R:127:PRO:HD3	2.36	0.56
1:R:145:GLU:CG	1:R:145:GLU:O	2.53	0.56
1:B:137:ASN:HB3	1:B:170:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:GLU:H	1:D:254:GLU:CD	2.08	0.56
1:G:319:GLU:HB3	1:G:324:LEU:HB2	1.86	0.56
1:H:56:GLN:HG2	1:H:60:ARG:NH1	2.20	0.56
1:L:24:ARG:HG3	1:L:25:GLN:N	2.19	0.56
1:L:258:ARG:O	1:L:261:GLU:HB2	2.06	0.56
1:P:246:SER:HA	1:P:249:SER:OG	2.05	0.56
1:R:248:LEU:HD12	1:R:275:VAL:HG22	1.88	0.56
1:B:99:ILE:CD1	1:E:120:ALA:HA	2.36	0.56
1:H:281:ARG:HH11	1:H:281:ARG:HG3	1.70	0.56
1:L:205:THR:CG2	1:L:207:LEU:H	2.18	0.56
1:M:200:PRO:HA	1:M:203:TYR:CZ	2.41	0.56
1:M:45:ILE:C	1:M:47:VAL:H	2.10	0.56
1:R:165:TYR:CB	1:R:321:ALA:HB1	2.32	0.56
4:G:1003:AMP:H5'1	4:G:1003:AMP:C8	2.35	0.56
1:I:19:TYR:O	1:I:24:ARG:HB3	2.06	0.56
1:K:281:ARG:N	1:K:282:PRO:CD	2.69	0.56
1:P:26:PHE:HA	1:P:29:LEU:HB2	1.88	0.56
1:R:184:MSE:HE3	1:R:192:LYS:HB3	1.88	0.56
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.89	0.55
1:M:105:MSE:HA	1:M:149:GLN:NE2	2.22	0.55
1:M:125:TYR:N	1:M:126:PRO:CD	2.69	0.55
1:M:161:PHE:CE2	1:M:169:PHE:HE2	2.24	0.55
1:P:133:ILE:O	1:P:138:THR:HG23	2.05	0.55
1:B:137:ASN:HA	1:B:170:THR:CG2	2.35	0.55
1:B:252:SER:O	1:B:255:GLU:HB2	2.05	0.55
1:J:26:PHE:CD2	1:J:29:LEU:HD12	2.41	0.55
1:K:238:ILE:CD1	1:K:268:PHE:CE2	2.89	0.55
1:Q:24:ARG:NH1	1:Q:24:ARG:HG2	2.21	0.55
1:B:281:ARG:HB3	1:B:282:PRO:HD3	1.87	0.55
1:G:278:GLU:HA	1:G:278:GLU:OE1	2.05	0.55
1:H:295:GLU:OE2	1:H:295:GLU:HA	2.05	0.55
1:I:101:GLU:O	1:I:105:MSE:HE2	2.06	0.55
1:M:228:ILE:HG22	1:M:228:ILE:O	2.05	0.55
1:E:133:ILE:O	1:E:138:THR:HG23	2.06	0.55
1:F:27:VAL:HG12	1:F:27:VAL:O	2.05	0.55
1:K:245:TYR:CD1	1:K:275:VAL:HG11	2.38	0.55
1:K:293:SER:OG	1:K:295:GLU:HB2	2.05	0.55
1:L:205:THR:HG22	1:L:207:LEU:H	1.72	0.55
1:M:40:VAL:O	1:M:40:VAL:HG23	2.07	0.55
1:N:141:VAL:HG12	1:N:143:VAL:HG13	1.88	0.55
1:O:55:ARG:NH1	1:R:324:LEU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:94:GLN:C	1:Q:97:VAL:HG12	2.25	0.55
1:R:105:MSE:HE1	1:R:150:HIS:CA	2.34	0.55
1:G:170:THR:O	1:G:172:PRO:HD3	2.06	0.55
1:K:150:HIS:O	1:K:154:THR:HG22	2.07	0.55
1:M:300:LEU:O	1:M:303:GLY:N	2.38	0.55
1:N:199:ASN:ND2	1:N:201:LYS:HB2	2.21	0.55
1:N:79:ILE:HB	1:N:82:GLU:HG3	1.87	0.55
1:O:175:ARG:HH21	1:O:175:ARG:CG	2.20	0.55
1:P:266:GLY:O	1:P:270:ALA:CB	2.54	0.55
1:R:241:LEU:HA	1:R:244:ILE:HD12	1.89	0.55
1:R:272:LEU:O	1:R:275:VAL:CG1	2.53	0.55
1:B:147:GLN:O	1:B:151:ILE:HG12	2.07	0.55
1:D:243:ASN:O	1:D:247:THR:OG1	2.25	0.55
1:H:288:HIS:O	1:H:292:GLU:HG2	2.06	0.55
1:I:26:PHE:HD2	1:I:26:PHE:N	2.04	0.55
1:L:164:ARG:HB3	1:L:165:TYR:CD2	2.42	0.55
1:M:126:PRO:CB	1:M:127:PRO:HD3	2.32	0.55
1:N:50:ASP:HB3	1:N:53:GLU:HG3	1.87	0.55
1:P:52:HIS:O	1:P:56:GLN:HG3	2.05	0.55
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.42	0.55
1:B:326:ARG:NH2	1:E:301:ASP:OD1	2.29	0.55
1:H:96:ILE:O	1:H:160:ARG:NH1	2.39	0.55
1:J:19:TYR:HB2	1:J:206:LEU:HD21	1.89	0.55
1:K:287:TYR:OH	1:K:291:MSE:CE	2.55	0.55
1:P:90:ALA:O	1:P:94:GLN:HG3	2.07	0.55
1:Q:176:ILE:CG1	1:Q:179:VAL:HB	2.36	0.55
1:R:29:LEU:HD22	1:R:33:TYR:CE1	2.42	0.55
1:B:260:TYR:CE1	1:B:271:ASP:OD2	2.59	0.55
1:E:145:GLU:O	1:E:145:GLU:HG3	2.06	0.55
1:M:64:LEU:HD21	1:M:207:LEU:HD21	1.88	0.55
1:M:213:ILE:HD11	1:M:280:LEU:HD12	1.89	0.55
1:N:101:GLU:O	1:N:105:MSE:HE2	2.07	0.55
1:P:169:PHE:CD1	1:P:314:MSE:HE3	2.42	0.55
1:P:241:LEU:HD22	1:P:272:LEU:HD23	1.89	0.55
1:P:86:HIS:HD2	1:P:132:ASP:OD1	1.90	0.55
1:R:18:ASN:ND2	4:R:1003:AMP:O4'	2.40	0.55
1:B:192:LYS:HE3	1:B:193:MSE:O	2.06	0.55
1:E:244:ILE:O	1:E:248:LEU:HB2	2.06	0.55
1:F:146:ASP:OD1	1:F:146:ASP:N	2.31	0.55
1:F:65:TYR:O	1:F:70:ILE:HB	2.06	0.55
1:G:129:MSE:O	1:G:132:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:LYS:N	3:H:1002:PO4:O2	2.29	0.55
1:H:175:ARG:O	1:H:177:PRO:HD3	2.07	0.55
1:K:191:LYS:HD2	1:K:192:LYS:N	2.21	0.55
1:K:238:ILE:CA	1:K:241:LEU:CD1	2.84	0.55
1:M:275:VAL:O	1:M:279:THR:OG1	2.24	0.55
1:Q:99:ILE:O	1:Q:103:GLU:HG3	2.07	0.55
1:A:55:ARG:HH22	1:D:320:GLN:NE2	2.05	0.55
1:B:106:THR:HB	1:B:149:GLN:OE1	2.07	0.55
1:C:43:HIS:HE1	1:C:132:ASP:OD2	1.90	0.55
1:F:304:ALA:O	1:F:308:ASN:HB2	2.07	0.55
1:I:145:GLU:O	1:I:148:LYS:HG2	2.06	0.55
1:Q:125:TYR:N	1:Q:126:PRO:CD	2.70	0.55
1:R:187:VAL:HG11	1:R:199:ASN:ND2	2.22	0.55
1:R:281:ARG:HB3	1:R:282:PRO:HD3	1.89	0.55
1:E:105:MSE:CA	1:E:105:MSE:HE2	2.36	0.54
1:M:313:GLU:OE2	1:M:316:ARG:NH2	2.40	0.54
1:M:41:ASP:OD1	1:M:80:GLN:HB3	2.08	0.54
1:P:289:HIS:O	1:P:293:SER:HB2	2.06	0.54
1:Q:125:TYR:CG	1:Q:126:PRO:HD3	2.42	0.54
1:Q:182:ARG:HA	4:Q:1003:AMP:H2	1.72	0.54
1:E:19:TYR:O	1:E:24:ARG:CB	2.55	0.54
1:I:249:SER:HB2	1:I:251:GLN:HG3	1.90	0.54
1:K:199:ASN:ND2	1:K:201:LYS:HB2	2.22	0.54
1:M:190:THR:HG22	1:M:191:LYS:N	2.22	0.54
1:M:22:ALA:O	1:M:25:GLN:HG2	2.07	0.54
1:M:19:TYR:HA	1:M:23:LEU:HB2	1.88	0.54
1:N:120:ALA:HB3	1:Q:97:VAL:HG12	1.88	0.54
1:O:24:ARG:NH2	1:O:247:THR:O	2.40	0.54
1:R:5:PHE:HE2	1:R:136:TYR:CE2	2.25	0.54
1:B:238:ILE:HG13	1:B:265:TYR:CE1	2.43	0.54
1:E:243:ASN:O	1:E:247:THR:HG23	2.07	0.54
1:H:253:ILE:O	1:H:253:ILE:CG2	2.56	0.54
1:J:213:ILE:HD11	1:J:280:LEU:HD12	1.90	0.54
1:P:182:ARG:NH1	1:P:192:LYS:HD2	2.22	0.54
1:P:241:LEU:HD23	1:P:244:ILE:CD1	2.36	0.54
1:P:280:LEU:C	1:P:282:PRO:HD2	2.28	0.54
1:O:118:VAL:HG12	1:R:99:ILE:CG1	2.37	0.54
1:A:199:ASN:HD22	1:A:200:PRO:CD	2.19	0.54
1:B:260:TYR:HE1	1:B:271:ASP:OD2	1.91	0.54
1:B:29:LEU:HD11	1:B:177:PRO:CB	2.27	0.54
1:C:129:MSE:HE3	2:C:1001:TRP:CZ3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1003:AMP:O1P	4:D:1003:AMP:H8	1.90	0.54
1:D:179:VAL:HG22	1:D:180:GLY:N	2.23	0.54
1:E:281:ARG:HB3	1:E:282:PRO:CD	2.37	0.54
1:F:294:GLU:HG3	1:F:294:GLU:O	2.07	0.54
1:I:141:VAL:HG12	1:I:143:VAL:HG13	1.89	0.54
1:K:199:ASN:HD22	1:K:201:LYS:H	1.54	0.54
1:M:5:PHE:CB	1:M:138:THR:HG21	2.37	0.54
4:N:1003:AMP:C5'	4:N:1003:AMP:C8	2.91	0.54
4:Q:1003:AMP:H5'1	4:Q:1003:AMP:H8	1.72	0.54
1:Q:94:GLN:CA	1:Q:97:VAL:HG12	2.36	0.54
1:R:244:ILE:O	1:R:248:LEU:HB2	2.08	0.54
1:D:126:PRO:HB2	1:D:127:PRO:CD	2.35	0.54
1:F:125:TYR:N	1:F:126:PRO:CD	2.70	0.54
1:L:98:TYR:HB2	1:L:101:GLU:HG3	1.89	0.54
1:N:71:ASP:HB3	1:N:74:GLN:HB2	1.89	0.54
1:P:15:THR:CG2	1:P:203:TYR:HB2	2.37	0.54
1:C:278:GLU:OE1	1:C:278:GLU:HA	2.07	0.54
1:F:59:ARG:HH11	1:F:59:ARG:CG	2.21	0.54
1:I:43:HIS:HE1	1:I:132:ASP:OD2	1.90	0.54
1:I:320:GLN:O	1:I:320:GLN:HG3	2.08	0.54
1:R:237:GLY:O	1:R:241:LEU:HD12	2.07	0.54
1:D:26:PHE:CD1	1:D:37:PHE:CE2	2.92	0.54
1:M:145:GLU:OE2	1:M:148:LYS:NZ	2.36	0.54
1:M:282:PRO:CB	1:M:286:ARG:NH2	2.67	0.54
1:N:29:LEU:HD22	1:N:33:TYR:CE1	2.42	0.54
1:O:72:PRO:HB3	1:O:299:VAL:CG1	2.37	0.54
1:Q:71:ASP:OD1	1:Q:72:PRO:HD2	2.08	0.54
1:A:278:GLU:HA	1:A:278:GLU:OE1	2.07	0.54
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.89	0.54
1:J:162:ASN:O	1:J:166:GLY:CA	2.55	0.54
1:K:239:SER:O	1:K:242:LEU:N	2.34	0.54
1:N:124:THR:HG21	1:Q:124:THR:HG21	1.90	0.54
1:O:24:ARG:HG2	1:O:24:ARG:NH1	2.22	0.54
1:O:26:PHE:HD2	1:O:29:LEU:CD1	2.08	0.54
1:E:119:SER:O	1:E:122:LEU:HB2	2.08	0.54
1:K:295:GLU:HG2	1:K:298:ARG:CZ	2.38	0.54
1:M:150:HIS:O	1:M:154:THR:HG23	2.08	0.54
1:M:199:ASN:ND2	1:M:201:LYS:H	2.05	0.54
1:M:289:HIS:HA	1:M:292:GLU:HG2	1.89	0.54
1:A:200:PRO:HA	1:A:203:TYR:CZ	2.43	0.54
1:B:133:ILE:O	1:B:138:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HG12	1:E:118:VAL:O	2.07	0.54
1:E:125:TYR:N	1:E:126:PRO:CD	2.71	0.54
1:E:152:GLU:HA	1:E:152:GLU:OE1	2.08	0.54
1:E:237:GLY:O	1:E:241:LEU:CD2	2.56	0.54
1:K:134:LEU:HB3	1:K:169:PHE:HE1	1.63	0.54
1:M:105:MSE:HE2	1:M:150:HIS:HE1	1.69	0.54
1:O:200:PRO:HA	1:O:203:TYR:CE2	2.43	0.54
1:M:164:ARG:NH2	1:P:48:TRP:CE3	2.76	0.54
1:Q:50:ASP:OD1	1:Q:51:PRO:HD2	2.08	0.54
1:B:190:THR:O	1:B:190:THR:CG2	2.56	0.53
1:F:5:PHE:HB2	1:F:138:THR:HG21	1.89	0.53
1:F:25:GLN:HG2	1:F:178:LYS:O	2.09	0.53
1:G:281:ARG:N	1:G:282:PRO:HD2	2.23	0.53
1:H:281:ARG:HB3	1:H:282:PRO:CD	2.38	0.53
4:P:1003:AMP:O3P	4:P:1003:AMP:H4'	2.06	0.53
1:P:143:VAL:HG21	1:P:151:ILE:CD1	2.34	0.53
1:E:126:PRO:N	1:E:127:PRO:HD2	2.23	0.53
1:E:281:ARG:N	1:E:282:PRO:HD2	2.23	0.53
1:G:129:MSE:HE3	2:G:1001:TRP:CD2	2.43	0.53
1:H:19:TYR:CE2	1:H:24:ARG:HD3	2.43	0.53
1:M:4:ILE:HG23	1:M:140:ILE:HG22	1.90	0.53
1:P:192:LYS:HE3	4:P:1003:AMP:C2	2.43	0.53
1:P:253:ILE:CG2	1:P:257:GLU:OE1	2.56	0.53
1:P:8:ILE:HD12	1:P:65:TYR:OH	2.07	0.53
1:Q:193:MSE:HB3	4:Q:1003:AMP:N6	2.22	0.53
1:R:288:HIS:O	1:R:292:GLU:CG	2.54	0.53
1:A:148:LYS:HG2	1:A:148:LYS:O	2.08	0.53
1:A:41:ASP:OD2	1:A:81:SER:HB3	2.08	0.53
1:B:175:ARG:CG	1:B:176:ILE:N	2.66	0.53
4:C:1003:AMP:H8	4:C:1003:AMP:H5'2	1.73	0.53
1:C:199:ASN:C	1:C:199:ASN:HD22	2.11	0.53
1:H:20:ILE:HD11	1:H:248:LEU:HG	1.90	0.53
1:I:272:LEU:O	1:I:276:VAL:HG23	2.09	0.53
1:L:25:GLN:O	1:L:29:LEU:HG	2.08	0.53
1:M:175:ARG:NH1	1:M:177:PRO:CG	2.61	0.53
1:N:4:ILE:HG21	1:N:26:PHE:HE1	1.73	0.53
1:Q:133:ILE:O	1:Q:138:THR:HG23	2.08	0.53
1:Q:159:GLU:O	1:Q:163:LYS:HG3	2.09	0.53
1:D:319:GLU:HB3	1:D:324:LEU:HB2	1.89	0.53
1:I:26:PHE:CD2	1:I:26:PHE:N	2.75	0.53
1:K:126:PRO:CD	1:K:127:PRO:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:228:ILE:HD11	1:K:264:GLY:O	2.07	0.53
1:L:106:THR:OG1	1:L:107:GLN:NE2	2.41	0.53
1:R:214:GLU:HB3	1:R:273:ALA:CB	2.38	0.53
1:B:274:GLN:O	1:B:278:GLU:HB2	2.09	0.53
1:F:289:HIS:O	1:F:293:SER:HB3	2.08	0.53
1:M:22:ALA:O	1:M:26:PHE:HD2	1.91	0.53
1:N:22:ALA:O	1:N:26:PHE:CD2	2.61	0.53
1:N:274:GLN:O	1:N:278:GLU:HB2	2.09	0.53
1:N:281:ARG:HB3	1:N:282:PRO:CD	2.38	0.53
1:C:17:GLY:HA2	1:C:183:ILE:HG13	1.91	0.53
1:E:150:HIS:O	1:E:154:THR:CG2	2.57	0.53
1:E:308:ASN:O	1:E:312:SER:HB3	2.08	0.53
1:F:256:LEU:HD22	1:F:260:TYR:HE2	1.74	0.53
1:H:129:MSE:HG3	2:H:1001:TRP:CE2	2.44	0.53
1:O:195:LYS:CG	1:O:196:SER:N	2.72	0.53
1:O:19:TYR:CE2	1:O:24:ARG:CD	2.92	0.53
1:R:187:VAL:CG1	1:R:201:LYS:HB2	2.39	0.53
1:A:8:ILE:HD12	1:A:65:TYR:OH	2.08	0.53
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.44	0.53
1:C:72:PRO:HB3	1:C:299:VAL:HG13	1.91	0.53
1:E:40:VAL:O	1:E:40:VAL:HG23	2.08	0.53
1:G:8:ILE:HD12	1:G:65:TYR:OH	2.08	0.53
1:N:43:HIS:HE1	1:N:132:ASP:OD2	1.91	0.53
1:N:165:TYR:HB3	1:N:321:ALA:HB1	1.91	0.53
1:O:125:TYR:N	1:O:126:PRO:CD	2.70	0.53
1:O:86:HIS:HE1	1:O:136:TYR:OH	1.91	0.53
1:P:248:LEU:HD12	1:P:248:LEU:H	1.70	0.53
1:R:40:VAL:HG23	1:R:40:VAL:O	2.09	0.53
1:O:118:VAL:CG1	1:R:99:ILE:HD11	2.35	0.53
1:B:118:VAL:HG12	1:E:99:ILE:HD12	1.90	0.53
1:G:39:ILE:HG23	1:G:61:LEU:HD23	1.91	0.53
1:Q:26:PHE:O	1:Q:30:GLN:HB3	2.09	0.53
1:R:19:TYR:CZ	1:R:24:ARG:HG2	2.43	0.53
1:E:73:THR:OG1	1:E:74:GLN:N	2.41	0.53
1:F:199:ASN:ND2	1:F:201:LYS:H	2.06	0.53
1:H:199:ASN:C	1:H:199:ASN:ND2	2.62	0.53
1:M:48:TRP:C	1:M:49:GLN:HG2	2.28	0.53
1:M:71:ASP:O	1:M:75:ALA:N	2.34	0.53
1:N:182:ARG:O	1:N:184:MSE:HE2	2.08	0.53
1:B:199:ASN:HD22	1:B:199:ASN:C	2.11	0.53
1:G:176:ILE:O	1:G:179:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:PRO:HB3	1:H:299:VAL:HG13	1.90	0.53
1:K:287:TYR:CE1	1:K:291:MSE:HE2	2.43	0.53
1:K:8:ILE:N	1:K:8:ILE:HD13	2.23	0.53
1:L:128:LEU:O	1:L:128:LEU:HD12	2.09	0.53
1:M:205:THR:CG2	1:M:207:LEU:H	2.07	0.53
1:N:254:GLU:H	1:N:254:GLU:CD	2.12	0.53
1:P:126:PRO:HD2	1:P:127:PRO:HD2	1.90	0.53
1:R:205:THR:HG22	1:R:207:LEU:N	2.21	0.53
1:R:85:ALA:HB1	1:R:315:VAL:HG21	1.91	0.53
1:A:43:HIS:HE1	1:A:132:ASP:OD2	1.91	0.52
1:B:243:ASN:O	1:B:247:THR:OG1	2.25	0.52
1:B:40:VAL:O	1:B:40:VAL:HG23	2.09	0.52
1:C:8:ILE:HB	1:C:61:LEU:HD21	1.91	0.52
1:D:71:ASP:OD2	1:D:73:THR:OG1	2.26	0.52
1:G:40:VAL:O	1:G:40:VAL:HG23	2.08	0.52
1:G:78:PHE:CD1	1:G:78:PHE:N	2.77	0.52
1:G:224:SER:HB3	1:I:166:GLY:CA	2.37	0.52
1:J:182:ARG:O	1:J:184:MSE:HE2	2.09	0.52
1:L:26:PHE:CD1	1:L:37:PHE:HE2	2.27	0.52
1:O:131:ALA:O	1:O:135:LEU:HG	2.09	0.52
1:O:304:ALA:O	1:O:308:ASN:HB2	2.09	0.52
1:P:195:LYS:HB3	1:P:195:LYS:HZ2	1.74	0.52
1:O:301:ASP:OD1	1:R:326:ARG:NH2	2.40	0.52
1:A:147:GLN:O	1:A:151:ILE:HG12	2.09	0.52
1:B:39:ILE:HG23	1:B:61:LEU:HD23	1.91	0.52
1:C:30:GLN:O	1:C:74:GLN:HG3	2.09	0.52
1:E:107:GLN:OE1	1:E:150:HIS:NE2	2.42	0.52
1:F:42:GLN:HB2	1:F:80:GLN:OE1	2.08	0.52
1:G:224:SER:CB	1:I:166:GLY:CA	2.87	0.52
1:H:31:HIS:HA	1:H:74:GLN:NE2	2.24	0.52
1:G:320:GLN:NE2	1:J:55:ARG:HH22	2.08	0.52
1:M:182:ARG:NE	1:M:184:MSE:HE1	2.18	0.52
1:N:120:ALA:CB	1:Q:97:VAL:HG13	2.39	0.52
1:R:71:ASP:OD2	1:R:73:THR:OG1	2.27	0.52
1:B:255:GLU:HG3	1:B:258:ARG:NH2	2.24	0.52
1:C:125:TYR:N	1:C:126:PRO:CD	2.72	0.52
1:G:59:ARG:NH2	1:G:296:LEU:HD23	2.24	0.52
1:L:105:MSE:CE	1:L:150:HIS:CE1	2.91	0.52
1:O:175:ARG:NH2	1:O:177:PRO:CA	2.72	0.52
1:O:22:ALA:O	1:O:26:PHE:CE1	2.63	0.52
1:O:2:LYS:O	1:O:33:TYR:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:126:PRO:HD2	1:P:127:PRO:HD3	1.88	0.52
1:P:147:GLN:HA	1:P:150:HIS:HD2	1.75	0.52
1:R:252:SER:OG	1:R:255:GLU:N	2.43	0.52
1:B:59:ARG:NH2	1:B:296:LEU:HD23	2.24	0.52
1:D:150:HIS:O	1:D:154:THR:HG22	2.09	0.52
1:E:253:ILE:HG13	1:E:253:ILE:O	2.10	0.52
1:H:19:TYR:HA	1:H:23:LEU:HB3	1.90	0.52
1:N:72:PRO:HB3	1:N:299:VAL:HG13	1.91	0.52
1:B:141:VAL:HG12	1:B:143:VAL:HG13	1.92	0.52
1:D:281:ARG:HG3	1:D:281:ARG:NH1	2.25	0.52
1:F:106:THR:HG22	1:F:107:GLN:N	2.25	0.52
1:M:65:TYR:O	1:M:70:ILE:HG12	2.10	0.52
1:N:253:ILE:O	1:N:257:GLU:HG3	2.10	0.52
1:N:259:GLN:O	1:N:263:LYS:HE3	2.10	0.52
1:P:106:THR:O	1:P:106:THR:CG2	2.56	0.52
1:P:176:ILE:CB	1:P:179:VAL:CG2	2.65	0.52
1:A:125:TYR:N	1:A:126:PRO:CD	2.73	0.52
1:C:29:LEU:HD11	1:C:177:PRO:HB2	1.90	0.52
1:D:125:TYR:N	1:D:126:PRO:CD	2.72	0.52
1:O:25:GLN:HE21	1:O:25:GLN:H	1.56	0.52
1:P:161:PHE:O	1:P:161:PHE:CD2	2.63	0.52
1:P:295:GLU:OE1	1:P:298:ARG:NH2	2.43	0.52
1:F:133:ILE:O	1:F:138:THR:HG23	2.09	0.52
1:F:200:PRO:HA	1:F:203:TYR:CE2	2.45	0.52
1:H:72:PRO:CB	1:H:299:VAL:HG13	2.40	0.52
1:I:212:THR:HG22	1:I:216:LYS:HE3	1.92	0.52
1:J:313:GLU:HA	1:J:313:GLU:OE1	2.10	0.52
1:L:23:LEU:HD11	1:L:65:TYR:CE2	2.45	0.52
1:P:127:PRO:O	1:P:130:ALA:HB3	2.09	0.52
1:N:326:ARG:NH2	1:Q:301:ASP:OD1	2.43	0.52
3:E:1002:PO4:O2	4:E:1003:AMP:O5'	2.28	0.52
1:H:313:GLU:HA	1:H:313:GLU:OE1	2.10	0.52
1:I:125:TYR:N	1:I:126:PRO:CD	2.72	0.52
1:O:126:PRO:HB2	1:O:127:PRO:CD	2.40	0.52
1:Q:199:ASN:HD22	1:Q:200:PRO:HD2	1.75	0.52
1:D:26:PHE:O	1:D:30:GLN:HB3	2.10	0.52
1:E:290:TRP:CH2	1:E:299:VAL:HG21	2.44	0.52
1:N:59:ARG:CG	1:N:59:ARG:HH11	2.23	0.52
1:P:175:ARG:CG	1:P:176:ILE:N	2.73	0.52
1:P:18:ASN:C	1:P:18:ASN:ND2	2.56	0.52
1:P:295:GLU:O	1:P:299:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLN:NE2	1:A:25:GLN:H	2.07	0.52
1:C:242:LEU:HB3	1:C:253:ILE:HD13	1.91	0.52
1:E:238:ILE:O	1:E:241:LEU:N	2.43	0.52
1:G:60:ARG:HG2	1:G:287:TYR:OH	2.09	0.52
1:H:25:GLN:HG2	1:H:178:LYS:O	2.10	0.52
1:H:99:ILE:HG12	1:K:118:VAL:O	2.10	0.52
1:K:297:ASP:O	1:K:301:ASP:OD1	2.27	0.52
1:O:126:PRO:CD	1:O:127:PRO:HD2	2.39	0.52
1:P:125:TYR:C	1:P:127:PRO:HD2	2.30	0.52
1:P:253:ILE:O	1:P:257:GLU:N	2.43	0.52
1:P:295:GLU:OE1	1:P:298:ARG:NE	2.43	0.52
1:B:125:TYR:CD2	1:B:126:PRO:HD3	2.45	0.51
1:F:19:TYR:CE2	1:F:24:ARG:HG3	2.45	0.51
1:H:228:ILE:CD1	1:H:228:ILE:N	2.74	0.51
1:I:213:ILE:HD11	1:I:280:LEU:HD12	1.92	0.51
1:O:177:PRO:O	1:O:178:LYS:HB2	2.09	0.51
1:P:5:PHE:HB2	1:P:138:THR:HG21	1.91	0.51
1:R:241:LEU:HD12	1:R:241:LEU:H	1.74	0.51
1:E:301:ASP:O	1:E:305:GLU:HB2	2.11	0.51
1:F:59:ARG:HG3	1:F:59:ARG:HH11	1.76	0.51
1:G:182:ARG:O	1:G:184:MSE:HE2	2.10	0.51
1:G:18:ASN:ND2	4:G:1003:AMP:C5'	2.69	0.51
1:H:129:MSE:HE1	1:H:147:GLN:OE1	2.10	0.51
1:K:190:THR:CG2	1:K:190:THR:O	2.58	0.51
1:K:200:PRO:O	1:K:216:LYS:HE2	2.10	0.51
1:L:205:THR:HG22	1:L:207:LEU:N	2.25	0.51
1:N:151:ILE:HA	1:N:154:THR:HG23	1.91	0.51
1:O:183:ILE:N	4:O:1003:AMP:N1	2.56	0.51
1:Q:41:ASP:OD2	1:Q:81:SER:HB3	2.09	0.51
1:R:274:GLN:O	1:R:277:ILE:HB	2.10	0.51
1:R:280:LEU:HD23	1:R:280:LEU:N	2.24	0.51
1:C:146:ASP:OD1	1:C:146:ASP:N	2.39	0.51
1:C:53:GLU:OE2	1:C:53:GLU:HA	2.09	0.51
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.25	0.51
1:F:66:LEU:HD12	1:F:296:LEU:CD1	2.40	0.51
1:G:199:ASN:C	1:G:199:ASN:HD22	2.14	0.51
1:H:29:LEU:HD22	1:H:33:TYR:HE1	1.74	0.51
1:J:152:GLU:HA	1:J:152:GLU:OE1	2.10	0.51
1:L:151:ILE:HG13	1:L:174:ALA:HB2	1.91	0.51
1:P:238:ILE:HD13	1:P:268:PHE:CE2	2.45	0.51
1:O:91:TRP:HE1	1:R:42:GLN:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HB3	1:A:169:PHE:CE1	2.45	0.51
1:C:295:GLU:OE2	1:C:295:GLU:HA	2.10	0.51
1:E:38:CYS:SG	1:E:80:GLN:HB2	2.50	0.51
1:I:193:MSE:HE2	1:I:203:TYR:HA	1.93	0.51
1:I:24:ARG:CB	1:I:24:ARG:HH11	2.23	0.51
1:M:245:TYR:HB2	1:M:272:LEU:HD13	1.91	0.51
1:M:73:THR:OG1	1:M:74:GLN:N	2.44	0.51
1:O:297:ASP:O	1:O:301:ASP:OD1	2.29	0.51
1:P:184:MSE:H	1:P:240:ASN:ND2	2.08	0.51
1:R:187:VAL:HG22	1:R:202:ALA:HB1	1.84	0.51
1:R:19:TYR:CD2	1:R:24:ARG:CG	2.94	0.51
1:R:287:TYR:CE2	1:R:291:MSE:CG	2.94	0.51
1:R:287:TYR:CE2	1:R:291:MSE:HG2	2.45	0.51
1:E:164:ARG:HD3	1:E:165:TYR:CE2	2.46	0.51
1:E:9:GLN:NE2	1:E:9:GLN:HA	2.26	0.51
1:G:199:ASN:HD22	1:G:201:LYS:H	1.58	0.51
1:J:5:PHE:O	1:J:142:PRO:HD2	2.11	0.51
1:L:43:HIS:HE1	1:L:132:ASP:OD2	1.94	0.51
1:M:170:THR:O	1:M:172:PRO:HD3	2.11	0.51
1:Q:213:ILE:HD12	1:Q:277:ILE:HG13	1.92	0.51
1:Q:252:SER:OG	1:Q:254:GLU:HG2	2.09	0.51
1:H:23:LEU:HG	1:H:68:VAL:HG11	1.92	0.51
1:I:55:ARG:NH2	1:L:320:GLN:HE22	2.05	0.51
1:J:134:LEU:HB3	1:J:169:PHE:HD1	1.76	0.51
1:J:145:GLU:C	1:J:147:GLN:H	2.14	0.51
1:J:71:ASP:OD1	1:J:72:PRO:HD2	2.10	0.51
1:M:273:ALA:O	1:M:277:ILE:HG13	2.10	0.51
1:N:60:ARG:HG2	1:N:287:TYR:OH	2.09	0.51
1:O:213:ILE:HD12	1:O:277:ILE:HG12	1.92	0.51
3:P:1002:PO4:O1	4:P:1003:AMP:O1P	2.28	0.51
1:P:159:GLU:OE2	1:P:163:LYS:HE3	2.09	0.51
1:A:187:VAL:HG13	1:A:202:ALA:HA	1.92	0.51
1:B:171:ILE:N	1:B:171:ILE:HD13	2.26	0.51
1:C:105:MSE:HE2	1:C:105:MSE:CA	2.41	0.51
1:A:124:THR:CB	1:D:94:GLN:NE2	2.74	0.51
1:E:286:ARG:O	1:E:289:HIS:HB3	2.11	0.51
1:G:162:ASN:OD1	1:G:168:LEU:N	2.31	0.51
1:H:217:ILE:O	1:H:269:LYS:HE2	2.11	0.51
1:J:145:GLU:C	1:J:147:GLN:N	2.62	0.51
1:O:126:PRO:N	1:O:127:PRO:HD2	2.26	0.51
1:P:228:ILE:HD13	1:P:228:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:HG21	1:B:202:ALA:HB2	1.93	0.51
1:E:176:ILE:O	1:E:179:VAL:HG23	2.10	0.51
1:E:268:PHE:O	1:E:271:ASP:HB2	2.10	0.51
1:G:43:HIS:HE1	1:G:132:ASP:OD2	1.93	0.51
1:G:130:ALA:CB	1:G:154:THR:HB	2.40	0.51
1:G:313:GLU:HG3	1:G:317:LYS:HZ2	1.73	0.51
1:H:52:HIS:CE1	1:H:56:GLN:HE22	2.29	0.51
1:I:265:TYR:O	1:I:269:LYS:HG3	2.10	0.51
1:K:261:GLU:N	1:K:263:LYS:HD2	2.26	0.51
1:M:8:ILE:HD12	1:M:65:TYR:OH	2.10	0.51
1:P:151:ILE:HD12	1:P:174:ALA:CB	2.40	0.51
1:R:148:LYS:O	1:R:152:GLU:HG2	2.11	0.51
1:I:79:ILE:HB	1:I:82:GLU:HG3	1.93	0.51
1:K:155:ARG:NH1	1:K:171:ILE:CG2	2.74	0.51
1:K:165:TYR:CE1	1:K:322:MSE:HA	2.45	0.51
1:L:298:ARG:O	1:L:302:GLU:HB2	2.11	0.51
1:M:215:LYS:O	1:M:219:SER:OG	2.29	0.51
1:P:238:ILE:CD1	1:P:268:PHE:CE2	2.94	0.51
1:P:27:VAL:HG13	1:P:28:GLU:OE1	2.10	0.51
1:R:279:THR:C	1:R:282:PRO:HD2	2.30	0.51
1:R:295:GLU:HA	1:R:295:GLU:OE2	2.10	0.51
1:D:175:ARG:C	1:D:177:PRO:HD3	2.32	0.51
1:D:210:ALA:HA	1:D:277:ILE:HG12	1.92	0.51
1:J:106:THR:HG23	1:J:106:THR:O	2.10	0.51
1:K:271:ASP:O	1:K:275:VAL:CG1	2.59	0.51
1:O:215:LYS:O	1:O:219:SER:OG	2.29	0.51
1:P:17:GLY:HA2	1:P:183:ILE:HD12	1.93	0.51
1:R:162:ASN:HD21	1:R:169:PHE:H	1.59	0.51
1:R:43:HIS:CE1	1:R:132:ASP:OD2	2.64	0.51
1:G:199:ASN:ND2	1:G:201:LYS:H	2.08	0.50
1:H:86:HIS:HE1	1:H:136:TYR:OH	1.94	0.50
1:M:184:MSE:SE	1:M:192:LYS:HA	2.61	0.50
1:P:245:TYR:HA	1:P:272:LEU:HD12	1.93	0.50
1:Q:318:MSE:O	1:Q:322:MSE:HG3	2.11	0.50
1:A:182:ARG:O	1:A:184:MSE:HE2	2.12	0.50
1:H:45:ILE:HG21	1:K:322:MSE:HE2	1.93	0.50
1:I:5:PHE:CB	1:I:138:THR:HG21	2.41	0.50
1:M:141:VAL:N	1:M:173:GLU:O	2.43	0.50
1:N:3:THR:HB	1:N:138:THR:HA	1.92	0.50
1:O:187:VAL:HG13	1:O:202:ALA:HA	1.93	0.50
1:Q:319:GLU:HG2	1:Q:324:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:187:VAL:CG1	1:R:199:ASN:ND2	2.75	0.50
1:B:238:ILE:CG1	1:B:265:TYR:CE1	2.95	0.50
1:B:23:LEU:HD12	1:B:23:LEU:O	2.12	0.50
1:B:252:SER:O	1:B:255:GLU:HB3	2.11	0.50
1:B:29:LEU:CD1	1:B:177:PRO:CB	2.75	0.50
1:B:313:GLU:O	1:B:317:LYS:HG3	2.10	0.50
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.24	0.50
1:D:151:ILE:O	1:D:155:ARG:HG3	2.12	0.50
1:F:182:ARG:NH1	1:F:192:LYS:CD	2.65	0.50
1:H:203:TYR:O	1:H:216:LYS:HD3	2.11	0.50
1:K:238:ILE:HD12	1:K:268:PHE:HE2	1.75	0.50
1:L:147:GLN:O	1:L:150:HIS:HB2	2.12	0.50
1:L:182:ARG:HG2	1:L:184:MSE:CE	2.42	0.50
1:O:193:MSE:CB	4:O:1003:AMP:N6	2.74	0.50
1:O:210:ALA:HB1	1:O:277:ILE:HD13	1.93	0.50
1:Q:19:TYR:HA	1:Q:23:LEU:HB3	1.93	0.50
1:R:86:HIS:CD2	1:R:132:ASP:OD1	2.60	0.50
1:C:86:HIS:HE1	1:C:136:TYR:OH	1.95	0.50
1:D:86:HIS:HE1	1:D:136:TYR:OH	1.94	0.50
1:D:193:MSE:HB3	4:D:1003:AMP:N6	2.25	0.50
4:I:1003:AMP:H8	4:I:1003:AMP:H5'1	1.77	0.50
1:L:125:TYR:CD2	1:L:126:PRO:HD3	2.46	0.50
1:L:185:SER:OG	1:L:187:VAL:HG22	2.11	0.50
1:M:94:GLN:HG3	1:M:127:PRO:HG2	1.93	0.50
1:P:254:GLU:OE1	1:P:254:GLU:N	2.44	0.50
1:B:159:GLU:O	1:B:163:LYS:HG3	2.11	0.50
1:D:281:ARG:HH11	1:D:281:ARG:HG3	1.76	0.50
1:E:194:SER:O	1:E:203:TYR:CD2	2.65	0.50
1:F:185:SER:CB	1:F:188:ASP:O	2.58	0.50
1:J:133:ILE:O	1:J:138:THR:HG23	2.11	0.50
1:J:22:ALA:O	1:J:25:GLN:HG2	2.10	0.50
1:K:122:LEU:O	1:K:125:TYR:CE1	2.63	0.50
1:M:100:GLY:O	1:M:104:ARG:HG3	2.11	0.50
1:M:43:HIS:CE1	1:M:128:LEU:HG	2.46	0.50
1:N:200:PRO:O	1:N:216:LYS:NZ	2.35	0.50
1:P:24:ARG:CB	1:P:24:ARG:HH11	2.24	0.50
1:A:130:ALA:CB	1:A:154:THR:HB	2.42	0.50
1:A:19:TYR:CZ	1:A:24:ARG:HD2	2.46	0.50
1:C:242:LEU:O	1:C:246:SER:HB3	2.11	0.50
1:H:253:ILE:O	1:H:253:ILE:HG22	2.11	0.50
1:J:159:GLU:O	1:J:163:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:THR:O	1:K:122:LEU:HD22	2.12	0.50
1:K:256:LEU:HD22	1:K:260:TYR:CE1	2.46	0.50
1:K:256:LEU:HD23	1:K:259:GLN:HG2	1.93	0.50
1:K:293:SER:HG	1:K:295:GLU:H	1.59	0.50
1:L:230:TYR:CD1	1:L:230:TYR:C	2.85	0.50
1:I:91:TRP:HE1	1:L:42:GLN:HB3	1.77	0.50
3:N:1002:PO4:O1	4:N:1003:AMP:O1P	2.30	0.50
1:P:254:GLU:OE2	1:P:257:GLU:OE1	2.30	0.50
1:C:21:GLY:O	1:C:25:GLN:NE2	2.45	0.50
1:A:124:THR:OG1	1:D:94:GLN:NE2	2.45	0.50
1:E:184:MSE:HE1	1:E:191:LYS:CA	2.41	0.50
1:F:23:LEU:HA	1:F:26:PHE:HD2	1.77	0.50
1:L:315:VAL:O	1:L:319:GLU:HG3	2.11	0.50
1:M:281:ARG:CG	1:M:281:ARG:NH1	2.70	0.50
1:P:184:MSE:H	1:P:240:ASN:HD21	1.59	0.50
1:P:199:ASN:ND2	1:P:201:LYS:HB2	2.26	0.50
1:Q:92:MSE:O	1:Q:96:ILE:HG23	2.12	0.50
1:R:313:GLU:OE2	1:R:316:ARG:NE	2.45	0.50
1:B:126:PRO:HB2	1:B:127:PRO:CD	2.36	0.50
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.42	0.50
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.95	0.50
1:G:101:GLU:OE2	1:G:160:ARG:NH2	2.44	0.50
1:K:164:ARG:HG2	1:K:165:TYR:CE2	2.46	0.50
1:L:92:MSE:O	1:L:96:ILE:HG23	2.12	0.50
1:M:281:ARG:H	1:M:282:PRO:HD2	1.77	0.50
1:N:29:LEU:CD1	1:N:177:PRO:HB2	2.37	0.50
1:O:253:ILE:CG2	1:O:257:GLU:OE2	2.60	0.50
1:P:198:PRO:O	1:P:200:PRO:HD3	2.12	0.50
1:A:94:GLN:HE22	1:D:94:GLN:NE2	2.04	0.50
1:C:8:ILE:O	1:C:40:VAL:HG22	2.12	0.50
1:D:165:TYR:CZ	1:D:322:MSE:HG2	2.47	0.50
1:B:326:ARG:NH1	1:E:297:ASP:HA	2.27	0.50
1:F:124:THR:O	1:F:127:PRO:HD2	2.12	0.50
1:F:185:SER:O	1:F:188:ASP:O	2.30	0.50
1:G:100:GLY:O	1:G:104:ARG:HG3	2.11	0.50
1:J:150:HIS:O	1:J:154:THR:HG23	2.12	0.50
1:K:213:ILE:O	1:K:217:ILE:HG12	2.12	0.50
1:K:287:TYR:CZ	1:K:291:MSE:HE2	2.46	0.50
1:O:124:THR:HG21	1:R:124:THR:HG21	1.93	0.50
1:O:26:PHE:HA	1:O:29:LEU:HD12	1.93	0.50
1:P:213:ILE:CG2	1:P:217:ILE:HD12	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:9:GLN:HA	1:P:9:GLN:NE2	2.26	0.50
1:Q:182:ARG:NE	1:Q:184:MSE:HE1	2.27	0.50
1:B:137:ASN:CA	1:B:170:THR:CG2	2.90	0.49
1:B:199:ASN:HD22	1:B:200:PRO:CD	2.23	0.49
1:B:260:TYR:OH	1:B:271:ASP:OD2	2.30	0.49
1:H:272:LEU:HA	1:H:275:VAL:HG13	1.94	0.49
1:I:41:ASP:OD2	1:I:81:SER:HB3	2.12	0.49
1:K:238:ILE:HD11	1:K:268:PHE:CE2	2.47	0.49
1:L:213:ILE:HD11	1:L:280:LEU:HD12	1.93	0.49
1:O:193:MSE:H	4:O:1003:AMP:N6	2.10	0.49
1:O:193:MSE:N	4:O:1003:AMP:N6	2.60	0.49
1:P:213:ILE:HG23	1:P:276:VAL:HG11	1.94	0.49
1:Q:146:ASP:N	1:Q:146:ASP:OD1	2.32	0.49
1:R:267:VAL:O	1:R:267:VAL:HG12	2.12	0.49
1:A:200:PRO:HA	1:A:203:TYR:CE2	2.48	0.49
1:F:182:ARG:CZ	1:F:192:LYS:CG	2.89	0.49
1:H:295:GLU:O	1:H:298:ARG:N	2.42	0.49
4:K:1003:AMP:H8	4:K:1003:AMP:C5'	2.21	0.49
1:N:86:HIS:CD2	1:N:132:ASP:HA	2.46	0.49
1:O:141:VAL:HG12	1:O:143:VAL:HG13	1.93	0.49
1:B:139:ASP:HB2	1:B:140:ILE:HD12	1.95	0.49
1:B:175:ARG:HG3	1:B:176:ILE:H	1.72	0.49
1:B:22:ALA:HB1	1:B:26:PHE:HE2	1.77	0.49
1:C:133:ILE:O	1:C:138:THR:HG23	2.12	0.49
1:C:258:ARG:O	1:C:261:GLU:HG3	2.11	0.49
1:F:185:SER:HB3	1:F:188:ASP:HB3	1.92	0.49
3:G:1002:PO4:O2	4:G:1003:AMP:O2P	2.29	0.49
1:K:146:ASP:N	1:K:146:ASP:OD1	2.29	0.49
1:K:191:LYS:HD2	1:K:192:LYS:H	1.71	0.49
1:P:29:LEU:CD1	1:P:177:PRO:HB2	2.42	0.49
1:Q:199:ASN:C	1:Q:199:ASN:HD22	2.15	0.49
1:B:162:ASN:O	1:B:165:TYR:O	2.30	0.49
1:C:227:THR:HG22	1:C:229:ARG:HG3	1.94	0.49
1:A:118:VAL:O	1:D:98:TYR:HA	2.13	0.49
1:G:126:PRO:HB2	1:G:127:PRO:CD	2.37	0.49
1:J:129:MSE:HE3	2:J:1001:TRP:CZ3	2.47	0.49
1:J:211:LYS:O	1:J:215:LYS:HG2	2.13	0.49
1:J:26:PHE:CE2	1:J:29:LEU:HD12	2.48	0.49
1:N:126:PRO:HB2	1:N:127:PRO:CD	2.32	0.49
1:R:184:MSE:HE2	1:R:191:LYS:O	2.13	0.49
1:B:29:LEU:HD13	1:B:177:PRO:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:O	1:C:26:PHE:HE2	1.92	0.49
1:F:101:GLU:O	1:F:105:MSE:HE3	2.12	0.49
1:K:105:MSE:HE1	1:K:150:HIS:ND1	2.27	0.49
1:P:215:LYS:CE	1:P:215:LYS:O	2.61	0.49
1:P:41:ASP:OD2	1:P:81:SER:HB3	2.12	0.49
1:R:59:ARG:CG	1:R:59:ARG:HH11	2.26	0.49
1:B:238:ILE:HD11	1:B:265:TYR:CD1	2.48	0.49
1:B:281:ARG:CG	1:B:281:ARG:HH11	2.25	0.49
1:D:125:TYR:N	1:D:126:PRO:HD2	2.27	0.49
1:D:125:TYR:CD2	1:D:126:PRO:HD3	2.47	0.49
1:E:150:HIS:O	1:E:154:THR:HG23	2.12	0.49
1:F:96:ILE:O	1:F:160:ARG:NH1	2.44	0.49
1:J:59:ARG:CG	1:J:59:ARG:HH11	2.25	0.49
1:L:9:GLN:HG2	1:L:40:VAL:CG2	2.42	0.49
1:L:59:ARG:HH11	1:L:59:ARG:CG	2.25	0.49
1:M:267:VAL:HG13	1:Q:306:LYS:HA	1.93	0.49
1:N:39:ILE:HG23	1:N:61:LEU:HD23	1.95	0.49
1:O:128:LEU:O	1:O:132:ASP:OD1	2.31	0.49
1:P:16:ILE:HG21	1:P:204:ILE:HB	1.91	0.49
1:N:55:ARG:NH2	1:Q:320:GLN:NE2	2.60	0.49
1:B:205:THR:HG22	1:B:208:ASP:H	1.75	0.49
1:B:71:ASP:O	1:B:75:ALA:N	2.40	0.49
1:E:170:THR:O	1:E:172:PRO:HD3	2.12	0.49
1:F:92:MSE:O	1:F:96:ILE:HG23	2.13	0.49
1:G:212:THR:HG22	1:G:216:LYS:HE3	1.94	0.49
1:I:18:ASN:ND2	4:I:1003:AMP:O4'	2.45	0.49
1:M:292:GLU:HG3	1:M:293:SER:N	2.28	0.49
1:N:54:LEU:O	1:N:58:ILE:HG13	2.12	0.49
1:E:48:TRP:HB2	1:O:188:ASP:OD1	2.13	0.49
1:R:18:ASN:HD21	4:R:1003:AMP:H5'1	1.77	0.49
1:A:199:ASN:HD21	1:A:201:LYS:HG3	1.78	0.49
1:A:59:ARG:HH11	1:A:59:ARG:CG	2.26	0.49
1:J:27:VAL:HG12	1:J:27:VAL:O	2.13	0.49
1:K:19:TYR:O	1:K:24:ARG:HB3	2.13	0.49
1:N:228:ILE:CD1	1:N:265:TYR:HD1	2.26	0.49
1:O:171:ILE:CD1	1:O:171:ILE:N	2.76	0.49
1:Q:26:PHE:HA	1:Q:29:LEU:HB2	1.95	0.49
1:R:162:ASN:O	1:R:166:GLY:O	2.31	0.49
1:R:41:ASP:CB	1:R:58:ILE:HD11	2.39	0.49
1:C:118:VAL:HB	1:F:99:ILE:HG13	1.93	0.49
1:C:5:PHE:CB	1:C:138:THR:HG21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HG12	1:F:118:VAL:O	2.13	0.49
1:D:228:ILE:HD11	1:D:265:TYR:HD1	1.78	0.49
1:F:105:MSE:HE2	1:F:105:MSE:N	2.28	0.49
1:H:72:PRO:HB3	1:H:299:VAL:CG1	2.42	0.49
1:I:176:ILE:HG12	1:I:179:VAL:HG13	1.91	0.49
1:L:80:GLN:NE2	1:L:132:ASP:OD1	2.43	0.49
1:M:175:ARG:HH12	1:M:177:PRO:CG	2.22	0.49
1:M:281:ARG:NH1	1:M:281:ARG:HB3	2.28	0.49
1:O:4:ILE:CG2	1:O:142:PRO:HD3	2.42	0.49
1:P:124:THR:O	1:P:127:PRO:HD2	2.13	0.49
1:N:99:ILE:CD1	1:Q:120:ALA:HA	2.42	0.49
1:N:99:ILE:HD13	1:Q:120:ALA:HA	1.93	0.49
1:R:56:GLN:OE1	1:R:57:ASN:ND2	2.46	0.49
1:A:195:LYS:HE2	3:A:1002:PO4:P	2.53	0.49
1:B:215:LYS:O	1:B:219:SER:OG	2.30	0.49
1:E:238:ILE:C	1:E:241:LEU:HD23	2.34	0.49
1:G:274:GLN:O	1:G:278:GLU:HB2	2.13	0.49
1:J:193:MSE:HE2	1:J:203:TYR:HA	1.94	0.49
1:J:320:GLN:O	1:J:320:GLN:HG3	2.13	0.49
1:K:155:ARG:HG2	1:K:171:ILE:HG23	1.95	0.49
1:O:193:MSE:CA	4:O:1003:AMP:HN61	2.25	0.49
1:O:5:PHE:CZ	1:O:38:CYS:HB2	2.48	0.49
1:P:245:TYR:CE2	1:P:256:LEU:HD13	2.46	0.49
1:A:159:GLU:HG3	1:A:163:LYS:HE2	1.95	0.48
1:B:245:TYR:O	1:B:245:TYR:HD1	1.95	0.48
1:C:212:THR:O	1:C:216:LYS:HB2	2.13	0.48
1:F:22:ALA:O	1:F:26:PHE:HD2	1.92	0.48
1:F:228:ILE:HD13	1:F:265:TYR:CE1	2.47	0.48
1:H:199:ASN:ND2	1:H:201:LYS:HB2	2.27	0.48
4:N:1003:AMP:H4'	4:N:1003:AMP:O3P	2.13	0.48
1:O:92:MSE:HB3	1:O:322:MSE:SE	2.63	0.48
1:Q:165:TYR:HB3	1:Q:321:ALA:HB1	1.95	0.48
1:R:53:GLU:OE2	1:R:56:GLN:NE2	2.45	0.48
1:C:295:GLU:O	1:C:299:VAL:HG23	2.13	0.48
1:J:197:ASP:OD1	1:J:198:PRO:HD2	2.13	0.48
1:J:315:VAL:HG12	1:J:316:ARG:N	2.27	0.48
1:M:209:ASP:O	1:M:213:ILE:HG13	2.14	0.48
1:M:278:GLU:OE1	1:M:278:GLU:HA	2.12	0.48
1:P:215:LYS:HE2	1:P:215:LYS:C	2.34	0.48
1:Q:150:HIS:O	1:Q:154:THR:HG22	2.13	0.48
1:Q:156:ASP:O	1:Q:160:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:238:ILE:CD1	1:Q:265:TYR:CE1	2.96	0.48
1:R:20:ILE:HG13	1:R:183:ILE:CD1	2.40	0.48
1:R:238:ILE:HA	1:R:241:LEU:CD1	2.43	0.48
1:A:289:HIS:O	1:A:293:SER:HB2	2.13	0.48
1:B:29:LEU:HD11	1:B:177:PRO:O	2.13	0.48
1:D:228:ILE:HD13	1:D:265:TYR:HE1	1.78	0.48
1:F:185:SER:C	1:F:188:ASP:O	2.52	0.48
1:H:22:ALA:O	1:H:26:PHE:HD2	1.94	0.48
1:I:91:TRP:NE1	1:L:42:GLN:HB3	2.29	0.48
1:M:195:LYS:C	1:M:197:ASP:H	2.16	0.48
1:N:304:ALA:O	1:N:308:ASN:HB2	2.13	0.48
1:P:298:ARG:NH1	1:P:298:ARG:HG3	2.28	0.48
1:Q:65:TYR:O	1:Q:70:ILE:HB	2.13	0.48
1:B:1:MSE:HE3	1:B:34:ASN:HB2	1.94	0.48
1:B:83:VAL:HG13	1:B:308:ASN:ND2	2.28	0.48
1:E:267:VAL:CG1	1:E:268:PHE:H	2.26	0.48
1:H:185:SER:HB2	1:H:202:ALA:HB1	1.95	0.48
1:M:71:ASP:OD1	1:M:73:THR:HG23	2.12	0.48
1:O:289:HIS:CG	1:O:290:TRP:N	2.81	0.48
1:Q:24:ARG:CG	1:Q:24:ARG:NH1	2.75	0.48
1:R:123:LEU:O	1:R:123:LEU:HG	2.11	0.48
1:D:146:ASP:N	1:D:146:ASP:OD1	2.30	0.48
1:D:205:THR:HG22	1:D:207:LEU:N	2.24	0.48
1:F:308:ASN:O	1:F:312:SER:HB2	2.14	0.48
1:G:260:TYR:OH	1:G:271:ASP:OD2	2.27	0.48
1:L:30:GLN:O	1:L:74:GLN:HG3	2.14	0.48
1:N:124:THR:O	1:N:127:PRO:HD2	2.12	0.48
1:O:193:MSE:O	4:O:1003:AMP:N7	2.47	0.48
1:R:3:THR:HB	1:R:138:THR:HA	1.95	0.48
1:R:240:ASN:O	1:R:243:ASN:HB2	2.11	0.48
1:E:42:GLN:HB2	1:E:80:GLN:OE1	2.13	0.48
1:F:126:PRO:N	1:F:127:PRO:CD	2.77	0.48
1:C:320:GLN:HE22	1:F:55:ARG:NH2	2.07	0.48
1:H:19:TYR:HB2	1:H:206:LEU:HD11	1.94	0.48
1:H:84:PRO:HD2	1:H:308:ASN:HD21	1.78	0.48
1:I:136:TYR:HB2	1:I:138:THR:HG22	1.95	0.48
1:L:23:LEU:HD13	1:L:65:TYR:CE2	2.46	0.48
1:P:16:ILE:CG1	1:P:17:GLY:N	2.76	0.48
1:P:72:PRO:HB3	1:P:299:VAL:HG13	1.95	0.48
1:Q:188:ASP:HB3	1:Q:191:LYS:HB3	1.95	0.48
1:R:71:ASP:OD2	1:R:74:GLN:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HA	1:D:154:THR:HG23	1.95	0.48
1:A:325:GLY:O	1:D:55:ARG:HD2	2.12	0.48
1:G:150:HIS:O	1:G:154:THR:CG2	2.61	0.48
1:H:27:VAL:O	1:H:30:GLN:HG2	2.14	0.48
1:J:199:ASN:HD22	1:J:200:PRO:HD2	1.78	0.48
1:H:119:SER:HA	1:K:97:VAL:O	2.14	0.48
1:O:254:GLU:N	1:O:254:GLU:OE1	2.47	0.48
1:O:29:LEU:O	1:O:32:GLU:N	2.41	0.48
1:Q:140:ILE:CD1	1:Q:175:ARG:O	2.61	0.48
1:N:120:ALA:CB	1:Q:97:VAL:CG1	2.91	0.48
1:R:19:TYR:CD2	1:R:24:ARG:CD	2.96	0.48
1:R:237:GLY:O	1:R:241:LEU:CD1	2.62	0.48
1:A:273:ALA:O	1:A:277:ILE:HG13	2.14	0.48
1:D:130:ALA:CB	1:D:154:THR:HB	2.44	0.48
1:D:282:PRO:O	1:D:286:ARG:HG3	2.14	0.48
1:E:245:TYR:O	1:E:245:TYR:HD1	1.97	0.48
1:L:185:SER:OG	1:L:187:VAL:CG2	2.62	0.48
1:P:212:THR:O	1:P:216:LYS:HB3	2.13	0.48
1:P:238:ILE:CD1	1:P:268:PHE:HE2	2.26	0.48
1:P:22:ALA:O	1:P:26:PHE:HD2	1.95	0.48
1:P:295:GLU:OE1	1:P:298:ARG:CZ	2.62	0.48
1:Q:199:ASN:HD22	1:Q:200:PRO:CD	2.27	0.48
1:R:124:THR:O	1:R:127:PRO:HD2	2.13	0.48
1:A:18:ASN:ND2	4:A:1003:AMP:H8	2.12	0.48
1:A:56:GLN:HG2	1:A:60:ARG:NH2	2.28	0.48
1:A:97:VAL:O	1:D:119:SER:HA	2.14	0.48
1:E:205:THR:CG2	1:E:207:LEU:H	2.15	0.48
1:E:84:PRO:HD2	1:E:308:ASN:HD21	1.78	0.48
1:F:213:ILE:HD11	1:F:280:LEU:HD12	1.95	0.48
1:J:120:ALA:O	1:J:124:THR:HG22	2.14	0.48
1:O:126:PRO:HD2	1:O:127:PRO:HD2	1.94	0.48
1:A:56:GLN:CG	1:A:60:ARG:NH2	2.76	0.48
1:B:143:VAL:HB	1:B:147:GLN:HB2	1.95	0.48
1:C:211:LYS:HE3	1:C:215:LYS:HD2	1.95	0.48
1:D:147:GLN:OE1	1:D:150:HIS:HD2	1.96	0.48
1:G:215:LYS:O	1:G:219:SER:OG	2.28	0.48
1:G:224:SER:CB	1:I:166:GLY:HA2	2.42	0.48
1:M:27:VAL:HB	1:M:28:GLU:OE1	2.14	0.48
1:M:84:PRO:HD2	1:M:308:ASN:HD21	1.79	0.48
1:P:151:ILE:CD1	1:P:174:ALA:HB1	2.42	0.48
1:A:162:ASN:HA	1:A:166:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CD2	1:B:132:ASP:HA	2.49	0.47
1:G:54:LEU:O	1:G:58:ILE:HG13	2.13	0.47
1:G:224:SER:CB	1:I:166:GLY:N	2.77	0.47
1:J:215:LYS:O	1:J:219:SER:OG	2.32	0.47
1:M:41:ASP:OD2	1:M:81:SER:HB3	2.13	0.47
1:O:133:ILE:HG23	1:O:138:THR:OG1	2.14	0.47
1:O:175:ARG:HH22	1:O:177:PRO:CG	2.26	0.47
1:O:184:MSE:HB3	1:O:191:LYS:O	2.14	0.47
1:Q:86:HIS:HD2	1:Q:132:ASP:OD1	1.97	0.47
1:R:272:LEU:CA	1:R:275:VAL:HG12	2.43	0.47
1:B:182:ARG:HA	4:B:1003:AMP:H2	1.78	0.47
1:C:42:GLN:HB3	1:F:91:TRP:HE1	1.79	0.47
1:E:293:SER:OG	1:E:295:GLU:HB2	2.14	0.47
1:E:313:GLU:CD	1:E:316:ARG:HE	2.18	0.47
1:E:71:ASP:OD1	1:E:72:PRO:HD2	2.15	0.47
1:F:313:GLU:OE1	1:F:313:GLU:HA	2.15	0.47
1:F:41:ASP:OD2	1:F:81:SER:HB3	2.13	0.47
1:M:140:ILE:CD1	1:M:175:ARG:HD3	2.44	0.47
1:M:199:ASN:HD22	1:M:201:LYS:H	1.62	0.47
1:P:182:ARG:HH11	1:P:192:LYS:HD2	1.79	0.47
1:P:225:GLU:CD	1:P:227:THR:OG1	2.52	0.47
1:P:245:TYR:HE1	1:P:271:ASP:O	1.97	0.47
1:R:5:PHE:CE2	1:R:136:TYR:CE2	3.02	0.47
1:R:187:VAL:HG23	1:R:188:ASP:N	2.29	0.47
1:B:273:ALA:O	1:B:277:ILE:HG13	2.15	0.47
1:D:304:ALA:O	1:D:308:ASN:HB2	2.14	0.47
1:D:83:VAL:HG13	1:D:308:ASN:HA	1.97	0.47
1:E:185:SER:N	1:E:191:LYS:O	2.36	0.47
1:G:213:ILE:O	1:G:217:ILE:HG12	2.13	0.47
1:J:168:LEU:HD11	1:J:317:LYS:HB3	1.95	0.47
1:J:318:MSE:O	1:J:322:MSE:HG3	2.14	0.47
1:K:167:GLU:HG2	1:K:167:GLU:O	2.13	0.47
1:L:23:LEU:CD1	1:L:65:TYR:CZ	2.97	0.47
1:L:258:ARG:O	1:L:259:GLN:C	2.51	0.47
1:M:214:GLU:OE1	1:Q:1:MSE:CE	2.62	0.47
1:O:59:ARG:NH2	1:O:296:LEU:HD23	2.28	0.47
1:R:151:ILE:HG13	1:R:174:ALA:HB2	1.95	0.47
1:R:313:GLU:OE2	1:R:316:ARG:NH2	2.47	0.47
1:A:89:ALA:HB2	1:A:135:LEU:HD21	1.96	0.47
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.97	0.47
1:M:185:SER:HG	1:M:188:ASP:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:281:ARG:N	1:M:282:PRO:CD	2.77	0.47
1:N:133:ILE:O	1:N:138:THR:HG23	2.14	0.47
1:O:25:GLN:O	1:O:29:LEU:HG	2.13	0.47
1:O:4:ILE:HD11	1:O:33:TYR:CG	2.48	0.47
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.97	0.47
1:B:213:ILE:HD12	1:B:277:ILE:HG12	1.95	0.47
1:F:179:VAL:HG12	1:F:180:GLY:O	2.14	0.47
1:F:215:LYS:O	1:F:219:SER:OG	2.29	0.47
4:I:1003:AMP:H8	4:I:1003:AMP:C5'	2.27	0.47
1:I:241:LEU:HB3	1:I:268:PHE:HE2	1.80	0.47
1:K:165:TYR:CD1	1:K:321:ALA:HB1	2.48	0.47
1:P:124:THR:C	1:P:127:PRO:HD2	2.35	0.47
1:Q:101:GLU:O	1:Q:105:MSE:HE3	2.15	0.47
1:Q:175:ARG:O	1:Q:175:ARG:HG3	2.14	0.47
1:Q:260:TYR:OH	1:Q:271:ASP:OD2	2.27	0.47
1:R:105:MSE:CE	1:R:150:HIS:ND1	2.78	0.47
4:A:1003:AMP:C8	4:A:1003:AMP:C5'	2.97	0.47
1:A:22:ALA:C	1:A:25:GLN:HE21	2.18	0.47
1:A:248:LEU:HD12	1:A:276:VAL:HG22	1.96	0.47
1:A:281:ARG:N	1:A:282:PRO:HD2	2.29	0.47
1:B:297:ASP:O	1:B:301:ASP:OD1	2.32	0.47
1:E:133:ILE:O	1:E:138:THR:CG2	2.62	0.47
1:F:59:ARG:CG	1:F:59:ARG:NH1	2.77	0.47
1:H:281:ARG:HB3	1:H:282:PRO:HD3	1.96	0.47
1:I:263:LYS:HD2	1:I:263:LYS:N	2.29	0.47
1:J:125:TYR:CD2	1:J:126:PRO:HD3	2.49	0.47
1:J:24:ARG:O	1:J:24:ARG:HG3	2.14	0.47
1:K:248:LEU:HD22	1:K:279:THR:HG21	1.96	0.47
1:O:19:TYR:CE1	1:O:68:VAL:HG13	2.40	0.47
1:A:105:MSE:CA	1:A:105:MSE:CE	2.86	0.47
1:B:107:GLN:NE2	1:B:107:GLN:H	2.13	0.47
1:C:194:SER:O	1:C:197:ASP:HB2	2.15	0.47
1:F:199:ASN:HD22	1:F:199:ASN:C	2.18	0.47
1:C:55:ARG:HD2	1:F:325:GLY:O	2.15	0.47
1:G:89:ALA:HB2	1:G:135:LEU:HD21	1.96	0.47
1:O:193:MSE:H	4:O:1003:AMP:HN62	1.61	0.47
1:O:217:ILE:HD11	1:O:276:VAL:HG21	1.96	0.47
1:P:185:SER:HB3	1:P:188:ASP:O	2.14	0.47
4:Q:1003:AMP:C8	4:Q:1003:AMP:H5'1	2.49	0.47
1:Q:56:GLN:O	1:Q:60:ARG:HB2	2.15	0.47
1:A:38:CYS:SG	1:A:80:GLN:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:O	1:B:276:VAL:HG23	2.14	0.47
1:C:137:ASN:ND2	1:C:170:THR:OG1	2.37	0.47
1:C:200:PRO:HA	1:C:203:TYR:CE2	2.50	0.47
1:E:248:LEU:HD13	1:E:279:THR:OG1	2.14	0.47
1:G:211:LYS:HG3	1:G:211:LYS:O	2.14	0.47
1:H:256:LEU:O	1:H:260:TYR:HD2	1.97	0.47
1:I:319:GLU:HG2	1:I:324:LEU:HD12	1.97	0.47
1:J:214:GLU:O	1:J:218:LYS:HG3	2.15	0.47
1:N:168:LEU:HD21	1:N:317:LYS:HD3	1.97	0.47
1:P:195:LYS:HB3	3:P:1002:PO4:O2	2.15	0.47
1:P:97:VAL:CG1	1:P:102:LEU:HD11	2.45	0.47
1:P:194:SER:HA	3:P:1002:PO4:O4	2.15	0.47
1:P:71:ASP:HB3	1:P:74:GLN:HB2	1.96	0.47
1:Q:107:GLN:NE2	1:Q:107:GLN:N	2.53	0.47
1:Q:203:TYR:O	1:Q:216:LYS:HD3	2.15	0.47
1:A:124:THR:CG2	1:D:124:THR:HG21	2.41	0.47
1:E:194:SER:HA	3:E:1002:PO4:O4	2.15	0.47
1:F:205:THR:CG2	1:F:207:LEU:N	2.70	0.47
1:C:128:LEU:HD22	1:F:91:TRP:CE2	2.50	0.47
1:H:158:ALA:HB3	1:H:171:ILE:HD12	1.95	0.47
1:H:137:ASN:ND2	1:H:170:THR:HG23	2.27	0.47
1:K:43:HIS:HE1	1:K:132:ASP:OD2	1.96	0.47
1:K:56:GLN:O	1:K:60:ARG:HG3	2.14	0.47
1:L:152:GLU:HA	1:L:152:GLU:OE1	2.14	0.47
1:M:96:ILE:O	1:M:160:ARG:NH2	2.48	0.47
1:N:192:LYS:NZ	3:N:1002:PO4:O3	2.48	0.47
1:Q:4:ILE:HG23	1:Q:140:ILE:HG23	1.97	0.47
1:A:86:HIS:HE1	1:A:136:TYR:OH	1.98	0.47
1:C:257:GLU:O	1:C:261:GLU:HG2	2.14	0.47
1:J:123:LEU:HG	1:J:123:LEU:O	2.15	0.47
1:J:3:THR:HB	1:J:138:THR:HA	1.97	0.47
1:K:184:MSE:HB2	1:K:240:ASN:OD1	2.14	0.47
1:K:228:ILE:CD1	1:K:260:TYR:HB3	2.45	0.47
1:M:25:GLN:O	1:M:29:LEU:HG	2.15	0.47
1:O:105:MSE:CE	1:O:105:MSE:CA	2.92	0.47
1:O:102:LEU:O	1:O:105:MSE:HB2	2.15	0.47
1:O:197:ASP:HA	1:O:198:PRO:HD3	1.75	0.47
1:P:228:ILE:CG2	1:P:268:PHE:CE2	2.98	0.47
1:R:56:GLN:HG2	1:R:60:ARG:HH21	1.80	0.47
1:A:320:GLN:NE2	1:D:55:ARG:HH21	2.06	0.47
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:CYS:O	1:J:119:SER:OG	2.29	0.47
1:H:315:VAL:O	1:H:319:GLU:HG3	2.15	0.47
1:H:42:GLN:HB2	1:H:80:GLN:OE1	2.14	0.47
1:I:25:GLN:OE1	1:I:178:LYS:O	2.33	0.47
1:J:124:THR:OG1	1:J:124:THR:O	2.32	0.47
4:M:1003:AMP:O3'	4:M:1003:AMP:O1P	2.29	0.47
4:M:1003:AMP:H3'	4:M:1003:AMP:P	2.55	0.47
4:N:1003:AMP:H2'	4:N:1003:AMP:H5'1	1.72	0.47
1:O:105:MSE:SE	1:O:149:GLN:HG2	2.65	0.47
1:O:228:ILE:O	1:O:228:ILE:HG22	2.13	0.47
1:O:213:ILE:HG21	1:O:276:VAL:CG1	2.45	0.47
1:R:5:PHE:CB	1:R:138:THR:HG21	2.44	0.47
1:R:56:GLN:CG	1:R:60:ARG:NH2	2.78	0.47
1:B:43:HIS:HE1	1:B:132:ASP:OD2	1.97	0.46
1:F:217:ILE:O	1:F:269:LYS:HE2	2.14	0.46
1:G:309:ARG:HB3	1:G:309:ARG:NH1	2.30	0.46
1:H:228:ILE:HD12	1:H:228:ILE:N	2.31	0.46
1:H:281:ARG:HG3	1:H:281:ARG:NH1	2.30	0.46
1:J:30:GLN:O	1:J:74:GLN:HG3	2.15	0.46
1:L:8:ILE:HD13	1:L:65:TYR:CE2	2.49	0.46
1:P:165:TYR:HB3	1:P:321:ALA:HB1	1.97	0.46
1:R:4:ILE:HG13	1:R:140:ILE:HB	1.97	0.46
1:R:205:THR:C	1:R:207:LEU:H	2.17	0.46
1:D:228:ILE:CD1	1:D:265:TYR:CD1	2.98	0.46
1:F:107:GLN:N	1:F:107:GLN:NE2	2.46	0.46
1:G:86:HIS:HD2	1:G:132:ASP:OD1	1.98	0.46
1:I:70:ILE:HD12	1:I:70:ILE:HA	1.70	0.46
1:K:124:THR:CA	1:K:126:PRO:HD2	2.45	0.46
1:M:126:PRO:HB2	1:M:127:PRO:CD	2.33	0.46
1:N:120:ALA:HB3	1:Q:97:VAL:HG13	1.97	0.46
1:N:253:ILE:HG22	1:N:254:GLU:N	2.31	0.46
1:O:319:GLU:HB3	1:O:324:LEU:HB2	1.96	0.46
1:O:85:ALA:HA	1:O:88:GLN:HG3	1.96	0.46
1:P:9:GLN:HE21	1:P:9:GLN:CA	2.23	0.46
1:R:205:THR:C	1:R:207:LEU:N	2.69	0.46
1:R:63:ALA:O	1:R:67:ALA:HB2	2.15	0.46
1:B:71:ASP:HB3	1:B:74:GLN:CB	2.44	0.46
1:D:5:PHE:O	1:D:142:PRO:HD2	2.16	0.46
1:I:278:GLU:OE1	1:I:281:ARG:NH2	2.49	0.46
1:J:274:GLN:O	1:J:278:GLU:HB2	2.16	0.46
1:K:295:GLU:CG	1:K:298:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:PHE:HB2	1:N:138:THR:HG21	1.97	0.46
1:P:238:ILE:HD13	1:P:268:PHE:HE2	1.80	0.46
1:R:213:ILE:HD13	1:R:277:ILE:HG12	1.92	0.46
1:B:205:THR:HG22	1:B:207:LEU:N	2.29	0.46
1:B:281:ARG:N	1:B:282:PRO:HD2	2.31	0.46
1:B:65:TYR:O	1:B:70:ILE:HB	2.15	0.46
1:D:228:ILE:CD1	1:D:265:TYR:HD1	2.27	0.46
1:G:125:TYR:CD2	1:G:126:PRO:HD3	2.51	0.46
1:G:199:ASN:HD21	1:G:201:LYS:HG3	1.80	0.46
1:J:130:ALA:CB	1:J:154:THR:HB	2.45	0.46
1:K:106:THR:CB	1:K:149:GLN:NE2	2.78	0.46
1:M:74:GLN:HE21	1:M:74:GLN:HA	1.81	0.46
1:O:175:ARG:NH2	1:O:175:ARG:CG	2.78	0.46
1:O:29:LEU:O	1:O:30:GLN:C	2.54	0.46
1:P:209:ASP:OD1	1:P:212:THR:OG1	2.30	0.46
1:C:227:THR:HG21	1:C:229:ARG:CZ	2.46	0.46
1:C:1:MSE:CG	1:D:211:LYS:HD2	2.29	0.46
1:F:297:ASP:O	1:F:301:ASP:OD1	2.33	0.46
1:H:158:ALA:HB3	1:H:171:ILE:CD1	2.45	0.46
1:I:225:GLU:HG3	1:N:163:LYS:HD3	1.98	0.46
1:J:5:PHE:HB2	1:J:138:THR:HG21	1.97	0.46
1:K:245:TYR:CE1	1:K:275:VAL:CG1	2.77	0.46
1:K:256:LEU:HD23	1:K:256:LEU:HA	1.79	0.46
1:K:272:LEU:HA	1:K:275:VAL:HG13	1.98	0.46
1:M:55:ARG:HH22	1:P:320:GLN:CD	2.18	0.46
1:Q:273:ALA:O	1:Q:277:ILE:HD12	2.16	0.46
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.73	0.46
1:C:155:ARG:O	1:C:159:GLU:HB2	2.16	0.46
1:D:254:GLU:CD	1:D:254:GLU:N	2.69	0.46
1:G:211:LYS:HD2	1:K:1:MSE:CG	2.45	0.46
1:K:40:VAL:O	1:K:40:VAL:HG23	2.15	0.46
1:L:289:HIS:O	1:L:293:SER:HB3	2.15	0.46
1:L:40:VAL:O	1:L:40:VAL:HG23	2.16	0.46
1:M:290:TRP:O	1:M:292:GLU:N	2.48	0.46
1:O:102:LEU:HD22	1:O:123:LEU:O	2.15	0.46
1:O:213:ILE:CG2	1:O:276:VAL:HG11	2.45	0.46
1:P:29:LEU:HD11	1:P:177:PRO:HB2	1.97	0.46
1:A:320:GLN:HE21	1:D:55:ARG:HH22	1.45	0.46
1:K:105:MSE:CE	1:K:150:HIS:CE1	2.99	0.46
1:M:161:PHE:CE2	1:M:169:PHE:CE2	3.02	0.46
1:N:159:GLU:O	1:N:163:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:ILE:HD11	1:N:265:TYR:HD1	1.81	0.46
1:O:165:TYR:HB3	1:O:321:ALA:HB1	1.98	0.46
1:P:245:TYR:CZ	1:P:275:VAL:HG21	2.42	0.46
4:Q:1003:AMP:C8	4:Q:1003:AMP:C5'	2.98	0.46
1:C:254:GLU:OE1	1:C:254:GLU:N	2.42	0.46
1:D:65:TYR:O	1:D:70:ILE:HB	2.16	0.46
4:E:1003:AMP:C5'	4:E:1003:AMP:C8	2.98	0.46
1:I:215:LYS:O	1:I:219:SER:OG	2.33	0.46
1:K:192:LYS:HB3	1:K:192:LYS:HE2	1.52	0.46
1:K:259:GLN:HG3	1:K:260:TYR:H	1.78	0.46
1:O:326:ARG:NH1	1:R:300:LEU:CB	2.79	0.46
1:O:33:TYR:N	1:O:33:TYR:CD1	2.84	0.46
1:P:193:MSE:HB3	4:P:1003:AMP:HN62	1.77	0.46
1:P:64:LEU:HG	1:P:287:TYR:CD1	2.51	0.46
1:Q:228:ILE:HG13	1:Q:260:TYR:HB3	1.98	0.46
1:R:184:MSE:CE	1:R:191:LYS:O	2.64	0.46
1:B:238:ILE:HD11	1:B:265:TYR:CE1	2.50	0.46
1:B:32:GLU:CG	1:B:33:TYR:CE1	2.99	0.46
1:E:9:GLN:HE21	1:E:9:GLN:HA	1.81	0.46
1:F:25:GLN:HB3	1:F:178:LYS:HB2	1.98	0.46
1:G:295:GLU:HG2	1:G:295:GLU:O	2.16	0.46
1:J:175:ARG:O	1:J:177:PRO:HD3	2.15	0.46
1:K:124:THR:O	1:K:127:PRO:HG2	2.14	0.46
1:M:161:PHE:HD2	1:M:169:PHE:CD2	2.34	0.46
1:O:3:THR:CG2	1:O:138:THR:HG22	2.43	0.46
1:O:71:ASP:OD2	1:O:73:THR:N	2.49	0.46
1:P:26:PHE:HZ	1:P:142:PRO:CB	2.29	0.46
1:P:4:ILE:HD12	1:P:33:TYR:CD2	2.51	0.46
4:R:1003:AMP:H8	4:R:1003:AMP:C5'	2.29	0.46
1:R:51:PRO:O	1:R:55:ARG:HB2	2.15	0.46
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.26	0.46
1:A:26:PHE:HA	1:A:29:LEU:HB2	1.98	0.46
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.84	0.46
1:D:38:CYS:SG	1:D:80:GLN:HB2	2.57	0.46
1:F:106:THR:O	1:F:107:GLN:C	2.53	0.46
1:G:197:ASP:C	1:G:199:ASN:H	2.20	0.46
1:G:197:ASP:C	1:G:199:ASN:N	2.69	0.46
1:H:101:GLU:CD	1:H:160:ARG:HH22	2.18	0.46
1:M:210:ALA:CB	1:M:277:ILE:CD1	2.80	0.46
1:N:20:ILE:HD13	1:N:247:THR:OG1	2.16	0.46
1:N:26:PHE:O	1:N:30:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:230:TYR:CD2	1:P:253:ILE:CD1	2.99	0.46
1:R:184:MSE:HE3	1:R:192:LYS:CB	2.46	0.46
1:R:257:GLU:O	1:R:260:TYR:C	2.54	0.46
1:A:242:LEU:O	1:A:246:SER:HB3	2.16	0.45
1:B:59:ARG:NH1	1:B:59:ARG:CG	2.79	0.45
1:N:185:SER:HB3	1:N:188:ASP:O	2.16	0.45
1:O:306:LYS:HG2	1:O:309:ARG:NH2	2.31	0.45
1:R:319:GLU:HB3	1:R:324:LEU:HB2	1.97	0.45
1:C:79:ILE:HB	1:C:82:GLU:HG3	1.97	0.45
1:E:126:PRO:N	1:E:127:PRO:CD	2.79	0.45
1:E:63:ALA:CB	1:E:291:MSE:SE	3.14	0.45
1:F:205:THR:HG22	1:F:207:LEU:H	1.66	0.45
1:F:245:TYR:CD1	1:F:256:LEU:HD11	2.51	0.45
1:F:245:TYR:CE1	1:F:256:LEU:HD21	2.51	0.45
1:G:169:PHE:HZ	1:G:318:MSE:HE3	1.82	0.45
1:O:4:ILE:HG22	1:O:142:PRO:HD3	1.98	0.45
1:O:18:ASN:OD1	4:O:1003:AMP:O4'	2.34	0.45
1:P:143:VAL:CG2	1:P:151:ILE:CD1	2.94	0.45
1:P:251:GLN:HG3	1:P:256:LEU:HD21	1.99	0.45
1:Q:295:GLU:HG2	1:Q:298:ARG:NH1	2.32	0.45
1:A:213:ILE:HD11	1:A:280:LEU:HD12	1.98	0.45
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.16	0.45
3:B:1002:PO4:O4	4:B:1003:AMP:O1P	2.35	0.45
1:E:19:TYR:O	1:E:24:ARG:HB2	2.15	0.45
1:H:199:ASN:ND2	1:H:201:LYS:N	2.54	0.45
1:M:208:ASP:O	1:M:284:GLN:NE2	2.48	0.45
1:N:197:ASP:HA	1:N:198:PRO:HD3	1.79	0.45
1:O:205:THR:HG23	1:O:207:LEU:H	1.73	0.45
1:P:101:GLU:O	1:P:105:MSE:CG	2.60	0.45
1:P:249:SER:CB	1:P:251:GLN:HG2	2.46	0.45
1:P:5:PHE:CE1	1:P:132:ASP:HB3	2.52	0.45
1:Q:238:ILE:HD11	1:Q:265:TYR:CD1	2.52	0.45
1:R:281:ARG:N	1:R:282:PRO:CD	2.79	0.45
1:B:120:ALA:HA	1:E:99:ILE:CG1	2.47	0.45
1:B:280:LEU:HA	1:B:283:ILE:HD12	1.97	0.45
1:C:192:LYS:HE3	4:C:1003:AMP:C5	2.51	0.45
1:C:213:ILE:O	1:C:217:ILE:HG13	2.16	0.45
1:F:191:LYS:HB3	1:F:191:LYS:HE2	1.62	0.45
1:F:281:ARG:N	1:F:282:PRO:HD2	2.31	0.45
1:I:165:TYR:HB3	1:I:321:ALA:HB1	1.98	0.45
1:K:86:HIS:HE1	1:K:136:TYR:OH	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:ASN:OD1	1:L:60:ARG:NH2	2.50	0.45
1:Q:140:ILE:CD1	1:Q:175:ARG:CZ	2.95	0.45
1:Q:155:ARG:HD2	1:Q:172:PRO:O	2.15	0.45
1:R:126:PRO:N	1:R:127:PRO:CD	2.80	0.45
1:R:210:ALA:O	1:R:214:GLU:HG3	2.17	0.45
1:A:59:ARG:HH11	1:A:59:ARG:HG3	1.82	0.45
1:F:136:TYR:HB2	1:F:138:THR:HG22	1.97	0.45
1:F:179:VAL:CG1	1:F:180:GLY:O	2.64	0.45
1:G:208:ASP:O	1:G:284:GLN:NE2	2.46	0.45
1:M:290:TRP:C	1:M:292:GLU:N	2.69	0.45
1:O:125:TYR:CD2	1:O:126:PRO:HD3	2.51	0.45
1:O:150:HIS:O	1:O:154:THR:HG23	2.16	0.45
1:O:271:ASP:O	1:O:275:VAL:HG13	2.17	0.45
1:R:193:MSE:HE2	1:R:203:TYR:HA	1.98	0.45
1:R:246:SER:HA	1:R:251:GLN:HB2	1.98	0.45
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.73	0.45
1:B:8:ILE:HD13	1:B:65:TYR:OH	2.16	0.45
1:D:136:TYR:HB2	1:D:138:THR:HG22	1.98	0.45
1:E:123:LEU:HG	1:E:123:LEU:O	2.17	0.45
1:I:105:MSE:HB2	1:I:105:MSE:HE2	1.78	0.45
1:M:164:ARG:NH2	1:P:48:TRP:CD2	2.84	0.45
1:O:74:GLN:HG3	1:O:74:GLN:O	2.17	0.45
1:P:238:ILE:O	1:P:242:LEU:HG	2.16	0.45
1:P:25:GLN:O	1:P:29:LEU:HG	2.17	0.45
1:Q:96:ILE:O	1:Q:160:ARG:NH2	2.49	0.45
1:R:24:ARG:NH1	1:R:247:THR:O	2.49	0.45
1:R:278:GLU:O	1:R:282:PRO:HD3	2.17	0.45
1:R:45:ILE:C	1:R:47:VAL:H	2.19	0.45
1:A:19:TYR:CE2	1:A:24:ARG:HD2	2.52	0.45
1:C:313:GLU:OE2	1:C:316:ARG:NH2	2.50	0.45
1:D:182:ARG:HD3	1:D:184:MSE:HE1	1.99	0.45
1:D:40:VAL:O	1:D:40:VAL:HG23	2.17	0.45
1:G:315:VAL:O	1:G:319:GLU:HG3	2.17	0.45
1:I:71:ASP:HA	1:I:72:PRO:HD2	1.84	0.45
1:L:122:LEU:HA	1:L:122:LEU:HD12	1.84	0.45
1:M:99:ILE:O	1:M:99:ILE:HG23	2.16	0.45
1:N:213:ILE:O	1:N:217:ILE:HG13	2.16	0.45
1:N:80:GLN:NE2	1:N:132:ASP:OD1	2.49	0.45
1:O:209:ASP:O	1:O:213:ILE:HG13	2.16	0.45
1:P:315:VAL:O	1:P:319:GLU:HG3	2.16	0.45
1:N:99:ILE:CG1	1:Q:118:VAL:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:192:LYS:HB3	1:Q:192:LYS:HE2	1.55	0.45
1:Q:24:ARG:HH11	1:Q:24:ARG:HG2	1.78	0.45
1:Q:278:GLU:OE1	1:Q:281:ARG:NH2	2.47	0.45
1:R:105:MSE:CE	1:R:150:HIS:HA	2.40	0.45
1:B:182:ARG:HA	4:B:1003:AMP:C2	2.52	0.45
1:D:19:TYR:O	1:D:24:ARG:CB	2.56	0.45
1:H:254:GLU:O	1:H:258:ARG:CG	2.52	0.45
1:H:226:GLY:HA2	1:H:265:TYR:CZ	2.52	0.45
1:H:49:GLN:O	1:K:164:ARG:NH2	2.45	0.45
1:I:123:LEU:O	1:I:123:LEU:HG	2.16	0.45
1:I:249:SER:HB2	1:I:251:GLN:CG	2.46	0.45
1:J:241:LEU:HA	1:J:241:LEU:HD12	1.71	0.45
1:M:78:PHE:N	1:M:78:PHE:CD1	2.85	0.45
1:R:275:VAL:HG13	1:R:276:VAL:H	1.82	0.45
1:E:151:ILE:HA	1:E:154:THR:HG23	1.98	0.45
1:I:260:TYR:HA	1:I:263:LYS:HG3	1.95	0.45
1:J:168:LEU:CD1	1:J:317:LYS:HD3	2.47	0.45
1:K:256:LEU:HD22	1:K:260:TYR:CD1	2.52	0.45
1:K:71:ASP:O	1:K:75:ALA:N	2.31	0.45
1:L:281:ARG:HB3	1:L:282:PRO:CD	2.46	0.45
1:M:120:ALA:HA	1:P:99:ILE:HD13	1.98	0.45
1:M:162:ASN:HA	1:M:166:GLY:O	2.17	0.45
1:P:181:ALA:CB	1:P:243:ASN:ND2	2.73	0.45
1:P:8:ILE:HB	1:P:61:LEU:HD21	1.98	0.45
1:P:99:ILE:H	1:P:99:ILE:HG12	1.29	0.45
1:R:155:ARG:O	1:R:159:GLU:HB2	2.17	0.45
1:R:225:GLU:CD	1:R:227:THR:CG2	2.81	0.45
1:R:302:GLU:O	1:R:306:LYS:HG3	2.17	0.45
1:A:200:PRO:O	1:A:216:LYS:NZ	2.50	0.45
1:A:25:GLN:CD	1:A:25:GLN:H	2.21	0.45
1:C:118:VAL:O	1:F:99:ILE:HG13	2.17	0.45
1:D:171:ILE:N	1:D:171:ILE:HD12	2.32	0.45
1:E:25:GLN:NE2	1:E:178:LYS:O	2.45	0.45
1:E:230:TYR:HB2	1:E:242:LEU:HD13	1.99	0.45
1:G:134:LEU:HB3	1:G:169:PHE:CE1	2.52	0.45
1:H:209:ASP:O	1:H:213:ILE:HG13	2.17	0.45
1:I:199:ASN:C	1:I:199:ASN:HD22	2.14	0.45
1:I:60:ARG:HG2	1:I:287:TYR:OH	2.17	0.45
1:J:162:ASN:O	1:J:166:GLY:N	2.50	0.45
1:L:59:ARG:NH1	1:L:59:ARG:CG	2.79	0.45
1:M:253:ILE:O	1:M:257:GLU:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:72:PRO:HG3	1:M:299:VAL:HG11	1.99	0.45
1:N:86:HIS:HD2	1:N:132:ASP:OD1	2.00	0.45
1:P:162:ASN:O	1:P:166:GLY:N	2.50	0.45
1:P:241:LEU:HB3	1:P:272:LEU:CD2	2.46	0.45
1:R:171:ILE:CD1	1:R:171:ILE:N	2.80	0.45
1:B:183:ILE:N	4:B:1003:AMP:N1	2.55	0.44
1:B:129:MSE:O	1:B:132:ASP:HB2	2.16	0.44
1:D:192:LYS:HB3	1:D:192:LYS:HE2	1.82	0.44
1:K:271:ASP:O	1:K:275:VAL:HG12	2.16	0.44
1:M:161:PHE:CD2	1:M:169:PHE:CD2	3.05	0.44
1:N:228:ILE:CD1	1:N:265:TYR:CD1	2.99	0.44
1:N:245:TYR:CD2	1:N:256:LEU:CD1	2.96	0.44
1:P:162:ASN:O	1:P:166:GLY:CA	2.65	0.44
1:P:245:TYR:CA	1:P:272:LEU:HD11	2.45	0.44
1:P:24:ARG:O	1:P:27:VAL:HG12	2.17	0.44
1:Q:26:PHE:HD2	1:Q:29:LEU:HD12	1.82	0.44
1:A:188:ASP:OD2	1:A:191:LYS:HB2	2.17	0.44
1:H:25:GLN:HG2	1:H:178:LYS:HB2	1.98	0.44
1:G:55:ARG:HD2	1:J:325:GLY:O	2.17	0.44
3:K:1002:PO4:O2	4:K:1003:AMP:O1P	2.36	0.44
1:M:124:THR:HG21	1:P:124:THR:HG21	1.98	0.44
1:O:119:SER:O	1:O:122:LEU:HB2	2.16	0.44
1:P:151:ILE:HG21	1:P:174:ALA:HB2	1.97	0.44
1:R:183:ILE:C	1:R:184:MSE:HG2	2.33	0.44
1:R:199:ASN:OD1	1:R:201:LYS:HB2	2.18	0.44
1:R:254:GLU:OE1	1:R:254:GLU:N	2.51	0.44
1:R:59:ARG:CG	1:R:59:ARG:NH1	2.81	0.44
1:R:83:VAL:HG13	1:R:308:ASN:ND2	2.32	0.44
1:B:8:ILE:CD1	1:B:65:TYR:CZ	3.00	0.44
1:C:228:ILE:O	1:C:229:ARG:HG2	2.18	0.44
1:H:197:ASP:HA	1:H:198:PRO:HD3	1.52	0.44
1:H:41:ASP:N	1:H:41:ASP:OD1	2.49	0.44
1:I:19:TYR:O	1:I:24:ARG:HB2	2.15	0.44
1:G:211:LYS:HD2	1:K:1:MSE:HG3	2.00	0.44
1:K:229:ARG:HG2	1:K:230:TYR:H	1.82	0.44
1:K:313:GLU:OE2	1:K:316:ARG:NH2	2.41	0.44
1:L:192:LYS:HE3	1:L:193:MSE:O	2.17	0.44
1:Q:140:ILE:HD12	1:Q:175:ARG:NE	2.33	0.44
1:R:287:TYR:CE2	1:R:291:MSE:HG3	2.52	0.44
1:A:277:ILE:O	1:A:281:ARG:HB2	2.16	0.44
1:B:20:ILE:HG22	1:B:20:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.67	0.44
1:C:22:ALA:O	1:C:26:PHE:HD2	1.97	0.44
1:C:260:TYR:HA	1:C:263:LYS:HG2	2.00	0.44
1:B:55:ARG:HD2	1:E:323:GLY:C	2.38	0.44
1:F:192:LYS:HB3	1:F:192:LYS:HE2	1.34	0.44
1:I:277:ILE:O	1:I:281:ARG:HB2	2.17	0.44
1:J:42:GLN:HB2	1:J:80:GLN:OE1	2.17	0.44
1:M:45:ILE:C	1:M:47:VAL:N	2.71	0.44
1:N:26:PHE:O	1:N:30:GLN:HB3	2.16	0.44
1:P:249:SER:OG	1:P:251:GLN:HG2	2.18	0.44
1:R:148:LYS:HB2	1:R:148:LYS:HE2	1.88	0.44
1:R:162:ASN:CA	1:R:166:GLY:O	2.64	0.44
1:R:19:TYR:CD2	1:R:24:ARG:HG3	2.53	0.44
1:F:184:MSE:CE	1:F:189:PRO:O	2.65	0.44
1:G:134:LEU:HB3	1:G:169:PHE:HD1	1.80	0.44
1:H:148:LYS:HE2	1:H:148:LYS:HB2	1.43	0.44
1:H:16:ILE:O	1:H:20:ILE:HB	2.18	0.44
1:H:253:ILE:O	1:H:257:GLU:HG3	2.17	0.44
1:K:8:ILE:HB	1:K:61:LEU:HD21	1.99	0.44
1:L:72:PRO:HB3	1:L:299:VAL:HG13	1.99	0.44
1:M:150:HIS:O	1:M:154:THR:CG2	2.65	0.44
1:M:48:TRP:O	1:M:49:GLN:HG2	2.18	0.44
1:O:195:LYS:HB3	1:O:195:LYS:HE3	1.57	0.44
1:O:209:ASP:OD1	1:O:209:ASP:N	2.50	0.44
1:P:94:GLN:HA	1:P:97:VAL:CG1	2.46	0.44
1:Q:182:ARG:O	1:Q:184:MSE:HE2	2.17	0.44
1:A:201:LYS:CB	1:A:201:LYS:NZ	2.81	0.44
1:B:5:PHE:HB2	1:B:138:THR:HG21	2.00	0.44
1:C:25:GLN:H	1:C:25:GLN:CD	2.21	0.44
1:C:50:ASP:HA	1:C:51:PRO:HD3	1.85	0.44
1:H:8:ILE:HB	1:H:61:LEU:HD21	2.00	0.44
1:H:96:ILE:HD13	1:H:96:ILE:N	2.32	0.44
1:I:119:SER:O	1:I:122:LEU:HB2	2.16	0.44
1:I:130:ALA:HB1	1:I:154:THR:HB	1.99	0.44
1:I:297:ASP:OD2	1:L:326:ARG:NH1	2.39	0.44
1:I:29:LEU:HD11	1:I:177:PRO:HB2	1.99	0.44
1:K:287:TYR:CZ	1:K:291:MSE:HE3	2.51	0.44
1:K:71:ASP:HA	1:K:72:PRO:HD2	1.81	0.44
1:L:5:PHE:CB	1:L:138:THR:HG21	2.43	0.44
1:N:199:ASN:HD22	1:N:201:LYS:H	1.65	0.44
1:N:40:VAL:HG23	1:N:40:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:59:ARG:CG	1:N:59:ARG:NH1	2.79	0.44
1:Q:43:HIS:HE1	1:Q:132:ASP:OD2	1.99	0.44
1:Q:151:ILE:HG21	1:Q:174:ALA:HB2	2.00	0.44
1:Q:215:LYS:HE2	1:Q:215:LYS:HB3	1.64	0.44
1:R:168:LEU:HA	1:R:168:LEU:HD23	1.82	0.44
1:R:56:GLN:HG2	1:R:60:ARG:NH2	2.32	0.44
1:A:125:TYR:N	1:A:126:PRO:HD2	2.32	0.44
1:E:141:VAL:HG12	1:E:143:VAL:HG13	2.00	0.44
1:B:118:VAL:HG12	1:E:99:ILE:CD1	2.48	0.44
1:L:182:ARG:HG2	1:L:184:MSE:HE1	2.00	0.44
1:L:313:GLU:HA	1:L:313:GLU:OE1	2.17	0.44
1:M:199:ASN:C	1:M:199:ASN:HD22	2.20	0.44
1:M:213:ILE:CD1	1:M:280:LEU:HD12	2.47	0.44
1:M:276:VAL:O	1:M:278:GLU:N	2.51	0.44
1:N:260:TYR:HA	1:N:263:LYS:HE3	2.00	0.44
1:O:205:THR:CG2	1:O:206:LEU:N	2.80	0.44
1:O:26:PHE:HA	1:O:29:LEU:HB2	1.99	0.44
1:P:218:LYS:HG2	1:P:219:SER:N	2.32	0.44
1:Q:199:ASN:HD22	1:Q:201:LYS:H	1.62	0.44
1:R:160:ARG:HG3	1:R:160:ARG:O	2.17	0.44
1:R:296:LEU:HA	1:R:296:LEU:HD12	1.71	0.44
1:A:130:ALA:HB1	1:A:154:THR:HB	2.00	0.44
1:A:106:THR:N	1:A:149:GLN:OE1	2.45	0.44
1:A:272:LEU:HA	1:A:275:VAL:HG13	1.99	0.44
4:B:1003:AMP:H8	4:B:1003:AMP:C5'	2.30	0.44
1:D:313:GLU:OE1	1:D:313:GLU:HA	2.18	0.44
1:G:59:ARG:NH1	1:G:297:ASP:OD1	2.44	0.44
1:I:176:ILE:O	1:I:176:ILE:HG13	2.18	0.44
1:I:278:GLU:CD	1:I:281:ARG:NH2	2.71	0.44
1:J:162:ASN:O	1:J:166:GLY:HA2	2.17	0.44
1:K:199:ASN:HA	1:K:200:PRO:HD2	1.80	0.44
1:K:230:TYR:CE1	1:K:239:SER:HB2	2.53	0.44
1:L:27:VAL:HG12	1:L:27:VAL:O	2.18	0.44
1:M:141:VAL:HA	1:M:142:PRO:HD2	1.90	0.44
1:O:183:ILE:HB	4:O:1003:AMP:N1	2.32	0.44
1:O:194:SER:O	1:O:197:ASP:HB2	2.18	0.44
1:B:238:ILE:HA	1:B:238:ILE:HD13	1.71	0.44
1:B:2:LYS:CD	1:B:2:LYS:N	2.80	0.44
1:B:40:VAL:HA	1:B:80:GLN:OE1	2.18	0.44
1:D:188:ASP:C	1:D:188:ASP:OD1	2.57	0.44
1:E:190:THR:CG2	1:O:48:TRP:CE3	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:O	1:E:216:LYS:HB2	2.18	0.44
1:F:25:GLN:CD	1:F:25:GLN:N	2.72	0.44
4:I:1003:AMP:C8	4:I:1003:AMP:C5'	3.01	0.44
1:L:241:LEU:HA	1:L:241:LEU:HD12	1.78	0.44
1:M:25:GLN:NE2	1:M:178:LYS:O	2.50	0.44
1:M:205:THR:CG2	1:M:206:LEU:N	2.81	0.44
1:N:228:ILE:HD13	1:N:265:TYR:CE1	2.52	0.44
1:N:251:GLN:OE1	1:N:259:GLN:NE2	2.47	0.44
1:O:91:TRP:NE1	1:R:42:GLN:HB3	2.33	0.44
1:Q:258:ARG:O	1:Q:261:GLU:HB3	2.17	0.44
1:Q:168:LEU:HD21	1:Q:317:LYS:HB3	2.00	0.44
1:R:60:ARG:HG3	1:R:287:TYR:OH	2.18	0.44
1:R:76:THR:HG23	1:R:306:LYS:HE3	2.00	0.44
1:A:225:GLU:O	1:A:227:THR:HG23	2.18	0.43
1:B:96:ILE:HD11	1:B:157:LEU:HD22	2.00	0.43
1:E:105:MSE:CA	1:E:105:MSE:CE	2.96	0.43
1:H:146:ASP:OD1	1:H:146:ASP:N	2.49	0.43
1:I:147:GLN:O	1:I:150:HIS:HB2	2.18	0.43
1:L:295:GLU:O	1:L:299:VAL:HG23	2.18	0.43
1:M:175:ARG:O	1:M:177:PRO:HD3	2.18	0.43
1:N:245:TYR:CD2	1:N:256:LEU:HD22	2.51	0.43
1:P:129:MSE:O	1:P:129:MSE:HG3	2.16	0.43
1:Q:157:LEU:HD21	1:Q:160:ARG:NH2	2.32	0.43
1:Q:281:ARG:N	1:Q:282:PRO:HD2	2.33	0.43
1:R:78:PHE:N	1:R:78:PHE:CD1	2.86	0.43
1:B:230:TYR:CD1	1:B:239:SER:CB	3.01	0.43
1:D:213:ILE:O	1:D:217:ILE:HG12	2.18	0.43
1:F:164:ARG:HE	1:F:164:ARG:HB2	1.60	0.43
1:G:17:GLY:HA2	1:G:183:ILE:HG13	2.00	0.43
1:H:158:ALA:CB	1:H:171:ILE:CD1	2.97	0.43
1:H:318:MSE:O	1:H:322:MSE:HG3	2.17	0.43
1:I:22:ALA:O	1:I:26:PHE:CD2	2.70	0.43
1:L:59:ARG:HH11	1:L:59:ARG:HG3	1.82	0.43
1:N:122:LEU:HA	1:N:122:LEU:HD13	1.71	0.43
1:O:126:PRO:CB	1:O:127:PRO:CD	2.96	0.43
1:P:216:LYS:CG	1:P:216:LYS:O	2.66	0.43
1:Q:238:ILE:HD11	1:Q:265:TYR:CE1	2.54	0.43
1:Q:281:ARG:HB3	1:Q:282:PRO:CD	2.48	0.43
1:R:228:ILE:CG1	1:R:260:TYR:HB3	2.47	0.43
1:B:254:GLU:O	1:B:258:ARG:CG	2.65	0.43
1:B:308:ASN:O	1:B:312:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PRO:N	1:C:127:PRO:HD2	2.33	0.43
1:C:199:ASN:HD22	1:C:200:PRO:N	2.16	0.43
1:C:201:LYS:HE3	1:C:201:LYS:HB3	1.57	0.43
1:D:168:LEU:CD2	1:D:314:MSE:SE	3.16	0.43
1:E:126:PRO:CB	1:E:127:PRO:CD	2.96	0.43
1:G:206:LEU:HD23	1:G:206:LEU:HA	1.84	0.43
1:I:193:MSE:HB3	4:I:1003:AMP:N6	2.33	0.43
1:J:176:ILE:HB	1:J:179:VAL:HG13	2.00	0.43
1:O:155:ARG:O	1:O:159:GLU:HB2	2.18	0.43
1:O:96:ILE:O	1:O:160:ARG:NH1	2.50	0.43
1:Q:106:THR:HG22	1:Q:107:GLN:N	2.33	0.43
1:Q:193:MSE:HE2	1:Q:203:TYR:HA	2.00	0.43
1:A:136:TYR:HB2	1:A:138:THR:HG22	2.00	0.43
1:C:188:ASP:HA	1:C:189:PRO:HD2	1.85	0.43
1:C:199:ASN:HD22	1:C:200:PRO:CD	2.31	0.43
1:E:107:GLN:H	1:E:107:GLN:HE21	1.65	0.43
1:F:176:ILE:HA	1:F:177:PRO:HD3	1.85	0.43
1:H:186:LEU:HB2	1:H:201:LYS:O	2.19	0.43
1:J:281:ARG:HB3	1:J:282:PRO:HD3	2.00	0.43
1:K:27:VAL:O	1:K:30:GLN:HG2	2.19	0.43
1:L:20:ILE:HD13	1:L:247:THR:OG1	2.18	0.43
1:L:210:ALA:HB1	1:L:277:ILE:HD13	2.00	0.43
1:M:147:GLN:O	1:M:150:HIS:HB2	2.18	0.43
1:M:211:LYS:HB2	1:Q:1:MSE:HG3	2.00	0.43
1:N:147:GLN:OE1	1:N:150:HIS:HD2	2.01	0.43
1:P:217:ILE:HD11	1:P:276:VAL:HG21	2.00	0.43
1:P:253:ILE:O	1:P:257:GLU:HB2	2.17	0.43
1:R:71:ASP:HA	1:R:72:PRO:HD2	1.81	0.43
1:R:94:GLN:HA	1:R:97:VAL:CG1	2.48	0.43
1:B:200:PRO:HA	1:B:203:TYR:CZ	2.54	0.43
1:C:241:LEU:HB3	1:C:268:PHE:HE2	1.84	0.43
1:E:19:TYR:O	1:E:24:ARG:HB3	2.19	0.43
1:F:20:ILE:HD13	1:F:247:THR:OG1	2.19	0.43
1:G:197:ASP:HA	1:G:198:PRO:HD2	1.73	0.43
1:G:213:ILE:HD11	1:G:280:LEU:HD12	2.01	0.43
1:H:150:HIS:O	1:H:154:THR:CG2	2.65	0.43
1:J:126:PRO:CB	1:J:127:PRO:HD3	2.44	0.43
1:N:278:GLU:OE1	1:N:278:GLU:HA	2.18	0.43
4:P:1003:AMP:H5'2	4:P:1003:AMP:N9	2.33	0.43
1:P:197:ASP:HA	1:P:198:PRO:HD2	1.81	0.43
1:P:245:TYR:CD1	1:P:272:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:HIS:O	1:C:56:GLN:HB2	2.19	0.43
1:F:136:TYR:HD1	1:F:310:VAL:HG11	1.84	0.43
1:H:195:LYS:HG2	3:H:1002:PO4:P	2.59	0.43
1:I:160:ARG:HB2	1:I:160:ARG:HE	1.73	0.43
1:I:25:GLN:OE1	1:I:176:ILE:HD11	2.19	0.43
1:I:42:GLN:HB2	1:I:80:GLN:OE1	2.19	0.43
1:J:185:SER:CA	1:J:188:ASP:O	2.66	0.43
1:K:239:SER:O	1:K:240:ASN:C	2.56	0.43
1:K:245:TYR:O	1:K:249:SER:N	2.52	0.43
1:K:258:ARG:CA	1:K:261:GLU:HG3	2.48	0.43
1:K:96:ILE:O	1:K:160:ARG:NH1	2.48	0.43
1:L:243:ASN:OD1	1:L:253:ILE:HD11	2.19	0.43
1:M:23:LEU:HD21	1:M:65:TYR:OH	2.18	0.43
1:M:64:LEU:HD21	1:M:287:TYR:CE1	2.54	0.43
1:N:295:GLU:O	1:N:299:VAL:HG23	2.19	0.43
1:P:228:ILE:CD1	1:P:228:ILE:N	2.82	0.43
1:Q:281:ARG:CG	1:Q:281:ARG:NH1	2.79	0.43
1:Q:59:ARG:CZ	1:Q:296:LEU:HD23	2.48	0.43
1:A:55:ARG:HD2	1:D:325:GLY:O	2.18	0.43
1:F:205:THR:HG22	1:F:208:ASP:N	2.34	0.43
1:G:151:ILE:HA	1:G:154:THR:HG23	2.01	0.43
1:I:89:ALA:HB2	1:I:135:LEU:HD21	1.99	0.43
1:J:125:TYR:CG	1:J:126:PRO:HD3	2.54	0.43
1:M:106:THR:H	1:M:149:GLN:HE22	1.67	0.43
1:O:19:TYR:HE1	1:O:68:VAL:CG1	2.25	0.43
1:P:218:LYS:CG	1:P:219:SER:N	2.80	0.43
1:P:298:ARG:HH11	1:P:298:ARG:HG3	1.82	0.43
1:R:29:LEU:HD22	1:R:33:TYR:HE1	1.82	0.43
1:A:59:ARG:NH1	1:A:59:ARG:CG	2.81	0.43
1:C:238:ILE:HA	1:C:238:ILE:HD13	1.77	0.43
1:F:32:GLU:HG2	1:F:32:GLU:H	1.64	0.43
1:H:86:HIS:CD2	1:H:132:ASP:HA	2.54	0.43
1:K:206:LEU:N	1:K:206:LEU:HD23	2.33	0.43
1:M:168:LEU:O	1:M:168:LEU:HD12	2.18	0.43
1:M:320:GLN:HE21	1:M:320:GLN:HB2	1.56	0.43
1:O:289:HIS:C	1:O:289:HIS:ND1	2.71	0.43
1:P:181:ALA:CB	1:P:243:ASN:HD22	2.11	0.43
1:B:32:GLU:HG2	1:B:33:TYR:CE1	2.54	0.43
1:B:8:ILE:CD1	1:B:65:TYR:OH	2.67	0.43
1:H:80:GLN:NE2	1:H:132:ASP:OD1	2.52	0.43
1:H:320:GLN:HA	1:K:55:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:SER:HA	1:K:242:LEU:HD12	2.01	0.43
1:L:238:ILE:HD13	1:L:238:ILE:HA	1.72	0.43
1:M:92:MSE:O	1:M:96:ILE:HG23	2.18	0.43
1:O:192:LYS:HG2	4:O:1003:AMP:N6	2.34	0.43
1:P:142:PRO:CA	1:P:175:ARG:O	2.40	0.43
1:P:249:SER:HB2	1:P:251:GLN:HG2	1.99	0.43
1:M:118:VAL:HB	1:P:99:ILE:CG1	2.48	0.43
1:R:213:ILE:O	1:R:217:ILE:HG13	2.19	0.43
1:C:41:ASP:N	1:C:41:ASP:OD1	2.52	0.43
1:D:210:ALA:HA	1:D:213:ILE:HD12	2.01	0.43
1:D:23:LEU:CD1	1:D:65:TYR:CE2	3.01	0.43
1:O:122:LEU:HA	1:O:122:LEU:HD12	1.87	0.43
4:P:1003:AMP:C5'	4:P:1003:AMP:N9	2.79	0.43
1:Q:40:VAL:HG23	1:Q:40:VAL:O	2.19	0.43
1:Q:94:GLN:HG2	1:Q:127:PRO:HG2	2.01	0.43
1:R:161:PHE:CD2	1:R:161:PHE:C	2.92	0.43
1:R:225:GLU:OE2	1:R:225:GLU:O	2.37	0.43
1:D:197:ASP:HA	1:D:198:PRO:HD3	1.83	0.42
1:E:106:THR:H	1:E:149:GLN:NE2	2.16	0.42
1:E:186:LEU:HD12	1:E:201:LYS:O	2.19	0.42
1:E:238:ILE:O	1:E:241:LEU:HD23	2.19	0.42
1:F:230:TYR:CD2	1:F:239:SER:HB3	2.54	0.42
1:G:71:ASP:HA	1:G:72:PRO:HD2	1.77	0.42
1:I:274:GLN:O	1:I:278:GLU:HB2	2.19	0.42
1:K:188:ASP:HA	1:K:189:PRO:HD2	1.84	0.42
1:M:293:SER:OG	1:M:294:GLU:N	2.52	0.42
1:N:55:ARG:HD2	1:Q:325:GLY:O	2.19	0.42
1:P:160:ARG:HB2	1:P:160:ARG:HE	1.59	0.42
1:P:267:VAL:CG2	1:P:268:PHE:N	2.82	0.42
1:M:55:ARG:HH22	1:P:320:GLN:HA	1.84	0.42
1:A:134:LEU:HB3	1:A:169:PHE:HD1	1.74	0.42
1:A:56:GLN:O	1:A:60:ARG:HG3	2.19	0.42
1:C:42:GLN:HB3	1:F:91:TRP:NE1	2.34	0.42
1:D:281:ARG:N	1:D:282:PRO:HD2	2.34	0.42
1:F:199:ASN:HD21	1:F:201:LYS:HB2	1.83	0.42
1:F:245:TYR:HH	1:F:260:TYR:HH	1.62	0.42
1:F:301:ASP:O	1:F:305:GLU:HB2	2.19	0.42
1:F:39:ILE:HG23	1:F:61:LEU:HD23	2.00	0.42
1:F:40:VAL:HG23	1:F:40:VAL:O	2.19	0.42
1:F:23:LEU:HD21	1:F:68:VAL:HG11	2.00	0.42
1:G:4:ILE:HD12	1:G:33:TYR:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:GLN:HG2	1:H:178:LYS:CB	2.49	0.42
1:I:125:TYR:CD2	1:I:126:PRO:HD3	2.53	0.42
1:J:197:ASP:HA	1:J:198:PRO:HD3	1.88	0.42
1:G:55:ARG:NH2	1:J:320:GLN:HA	2.33	0.42
1:K:165:TYR:CE1	1:K:321:ALA:O	2.72	0.42
1:K:134:LEU:CB	1:K:169:PHE:HE1	2.28	0.42
1:K:65:TYR:O	1:K:70:ILE:HB	2.20	0.42
4:L:1003:AMP:H8	4:L:1003:AMP:O1P	2.00	0.42
1:L:254:GLU:HA	1:L:257:GLU:OE1	2.19	0.42
1:M:185:SER:OG	1:M:187:VAL:CG2	2.63	0.42
1:N:59:ARG:HH11	1:N:59:ARG:HG3	1.84	0.42
1:B:289:HIS:C	1:B:289:HIS:ND1	2.72	0.42
1:C:71:ASP:HA	1:C:72:PRO:HD2	1.79	0.42
1:E:253:ILE:HA	1:E:256:LEU:HB3	2.01	0.42
1:E:287:TYR:C	1:E:289:HIS:H	2.23	0.42
1:G:101:GLU:CD	1:G:160:ARG:NH2	2.70	0.42
1:I:192:LYS:HG2	1:I:193:MSE:N	2.35	0.42
1:I:263:LYS:N	1:I:263:LYS:CD	2.80	0.42
1:O:280:LEU:O	1:O:284:GLN:HB2	2.20	0.42
1:P:39:ILE:HG12	1:P:61:LEU:HD23	2.00	0.42
1:R:106:THR:CB	1:R:149:GLN:HE22	2.32	0.42
1:R:214:GLU:CB	1:R:273:ALA:HB1	2.47	0.42
1:R:99:ILE:HG12	1:R:99:ILE:H	1.30	0.42
1:A:281:ARG:HB3	1:A:282:PRO:HD3	2.01	0.42
1:B:238:ILE:HG13	1:B:265:TYR:HE1	1.83	0.42
1:E:267:VAL:CG1	1:E:268:PHE:N	2.80	0.42
1:F:203:TYR:O	1:F:216:LYS:NZ	2.43	0.42
1:J:177:PRO:C	1:J:178:LYS:HG2	2.39	0.42
1:J:212:THR:CG2	1:J:216:LYS:HE3	2.49	0.42
1:J:319:GLU:HB3	1:J:324:LEU:HB2	2.02	0.42
1:M:203:TYR:O	1:M:216:LYS:NZ	2.46	0.42
1:N:281:ARG:N	1:N:282:PRO:HD2	2.35	0.42
1:O:182:ARG:HB3	1:O:184:MSE:HE1	2.01	0.42
1:Q:129:MSE:O	1:Q:132:ASP:HB2	2.20	0.42
1:Q:188:ASP:HA	1:Q:189:PRO:HD2	1.77	0.42
1:O:91:TRP:CZ2	1:R:128:LEU:HD22	2.55	0.42
1:R:215:LYS:HD2	1:R:215:LYS:C	2.39	0.42
4:B:1003:AMP:C8	4:B:1003:AMP:C5'	2.97	0.42
1:C:56:GLN:HB3	1:C:60:ARG:NH2	2.35	0.42
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.37	0.42
1:A:124:THR:CG2	1:D:94:GLN:HE22	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:PHE:CD1	1:E:37:PHE:CE2	3.06	0.42
1:E:279:THR:O	1:E:282:PRO:HG2	2.19	0.42
1:C:124:THR:HG21	1:F:124:THR:HG21	2.01	0.42
1:H:245:TYR:CD2	1:H:268:PHE:CE1	3.07	0.42
1:H:294:GLU:H	1:H:294:GLU:HG3	1.48	0.42
1:H:325:GLY:O	1:K:55:ARG:HD2	2.19	0.42
1:I:176:ILE:C	1:I:176:ILE:HD12	2.40	0.42
1:J:281:ARG:HB3	1:J:282:PRO:CD	2.50	0.42
1:K:129:MSE:O	1:K:132:ASP:HB2	2.19	0.42
1:L:281:ARG:HB3	1:L:282:PRO:HD3	2.00	0.42
1:M:199:ASN:CG	1:M:201:LYS:HG2	2.34	0.42
1:M:99:ILE:CG2	1:M:99:ILE:O	2.60	0.42
1:N:315:VAL:O	1:N:319:GLU:HG3	2.19	0.42
1:O:248:LEU:HD23	1:O:248:LEU:HA	1.56	0.42
1:O:326:ARG:HH12	1:R:300:LEU:CB	2.30	0.42
1:O:94:GLN:O	1:O:97:VAL:HG12	2.19	0.42
1:P:15:THR:HB	1:P:193:MSE:SE	2.70	0.42
1:P:253:ILE:O	1:P:257:GLU:CB	2.68	0.42
1:P:53:GLU:O	1:P:57:ASN:HB2	2.18	0.42
1:R:185:SER:OG	1:R:187:VAL:HG22	2.20	0.42
1:B:320:GLN:HE22	1:E:55:ARG:HH21	1.66	0.42
1:D:229:ARG:HB3	1:D:229:ARG:HE	1.67	0.42
1:E:26:PHE:HA	1:E:29:LEU:HB2	2.01	0.42
1:F:256:LEU:O	1:F:260:TYR:HD2	2.02	0.42
1:H:228:ILE:O	1:H:228:ILE:HG22	2.19	0.42
1:L:318:MSE:O	1:L:322:MSE:HG3	2.19	0.42
1:M:135:LEU:HD13	1:M:311:ALA:HB1	2.02	0.42
1:M:44:ALA:O	1:M:49:GLN:NE2	2.43	0.42
1:O:251:GLN:HB3	1:O:255:GLU:CD	2.40	0.42
1:O:213:ILE:HG23	1:O:276:VAL:HG11	2.01	0.42
1:P:168:LEU:HD23	1:P:168:LEU:HA	1.77	0.42
1:P:22:ALA:O	1:P:26:PHE:CD2	2.73	0.42
1:P:85:ALA:HB1	1:P:315:VAL:CG2	2.50	0.42
1:R:185:SER:OG	1:R:202:ALA:CB	2.55	0.42
1:C:126:PRO:CB	1:C:127:PRO:CD	2.95	0.42
1:E:9:GLN:HE21	1:E:9:GLN:CA	2.32	0.42
1:F:5:PHE:O	1:F:142:PRO:HD2	2.19	0.42
1:H:184:MSE:O	1:H:193:MSE:HE3	2.20	0.42
1:H:200:PRO:HA	1:H:203:TYR:CE2	2.55	0.42
1:K:268:PHE:CD1	1:K:268:PHE:O	2.73	0.42
1:L:214:GLU:O	1:L:218:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:THR:CB	1:L:94:GLN:NE2	2.82	0.42
1:M:5:PHE:HB2	1:M:138:THR:CG2	2.44	0.42
1:N:125:TYR:CG	1:N:126:PRO:HD3	2.55	0.42
1:O:225:GLU:O	1:O:227:THR:HG23	2.19	0.42
1:P:3:THR:HG22	1:P:138:THR:HB	2.00	0.42
1:R:106:THR:N	1:R:149:GLN:HE22	2.14	0.42
1:R:205:THR:O	1:R:207:LEU:N	2.53	0.42
1:R:272:LEU:CD1	1:R:272:LEU:C	2.84	0.42
1:A:71:ASP:HB3	1:A:74:GLN:CB	2.50	0.42
1:C:281:ARG:N	1:C:282:PRO:HD2	2.33	0.42
1:C:28:GLU:HA	1:C:31:HIS:CD2	2.44	0.42
1:E:29:LEU:CD1	1:E:177:PRO:HB2	2.48	0.42
1:E:66:LEU:HD13	1:E:290:TRP:CD2	2.55	0.42
1:G:285:GLU:OE1	1:G:285:GLU:HA	2.19	0.42
1:J:38:CYS:SG	1:J:80:GLN:HB2	2.60	0.42
1:K:258:ARG:O	1:K:261:GLU:CG	2.59	0.42
1:K:261:GLU:C	1:K:263:LYS:HD2	2.38	0.42
1:M:141:VAL:HG12	1:M:143:VAL:HG13	2.01	0.42
1:P:230:TYR:CD2	1:P:253:ILE:HD13	2.55	0.42
1:R:209:ASP:O	1:R:213:ILE:HG13	2.20	0.42
1:A:165:TYR:HB3	1:A:321:ALA:HB1	2.01	0.42
1:A:29:LEU:HD11	1:A:177:PRO:HB2	2.01	0.42
1:A:199:ASN:HA	1:A:200:PRO:HD3	1.83	0.42
1:E:106:THR:H	1:E:149:GLN:HE22	1.68	0.42
1:G:265:TYR:O	1:G:269:LYS:HG3	2.20	0.42
1:H:211:LYS:O	1:H:215:LYS:HG2	2.19	0.42
1:I:207:LEU:HD23	1:I:207:LEU:HA	1.89	0.42
1:L:15:THR:N	1:L:18:ASN:HD22	2.18	0.42
1:L:65:TYR:O	1:L:70:ILE:HB	2.20	0.42
1:M:210:ALA:HB2	1:M:277:ILE:HG23	2.02	0.42
1:O:201:LYS:HA	1:O:216:LYS:HE2	2.01	0.42
1:O:281:ARG:N	1:O:282:PRO:CD	2.83	0.42
1:P:97:VAL:HG21	1:P:102:LEU:HD21	2.01	0.42
1:R:281:ARG:HB3	1:R:282:PRO:CD	2.49	0.42
1:R:291:MSE:C	1:R:291:MSE:HE3	2.40	0.42
1:C:16:ILE:O	1:C:20:ILE:HG13	2.20	0.42
1:D:182:ARG:HG2	1:D:184:MSE:CE	2.49	0.42
1:E:3:THR:HG22	1:E:138:THR:HB	2.01	0.42
1:G:126:PRO:CB	1:G:127:PRO:CD	2.97	0.42
1:H:94:GLN:HG3	1:H:127:PRO:HG2	2.02	0.42
1:H:199:ASN:HD21	1:H:201:LYS:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:ASP:OD2	1:H:81:SER:HB3	2.19	0.42
1:I:92:MSE:O	1:I:96:ILE:HG23	2.20	0.42
1:J:130:ALA:HB1	1:J:154:THR:HB	2.00	0.42
1:J:304:ALA:O	1:J:308:ASN:HB2	2.19	0.42
1:K:56:GLN:NE2	1:K:56:GLN:CA	2.78	0.42
1:L:86:HIS:CD2	1:L:132:ASP:OD1	2.71	0.42
1:L:24:ARG:CG	1:L:24:ARG:HH11	2.33	0.42
1:M:276:VAL:O	1:M:279:THR:N	2.48	0.42
1:N:238:ILE:HD11	1:N:265:TYR:CD1	2.55	0.42
1:O:129:MSE:O	1:O:133:ILE:HD12	2.20	0.42
1:D:305:GLU:HB3	1:O:267:VAL:CG2	2.50	0.42
1:P:189:PRO:C	1:P:191:LYS:H	2.24	0.42
4:Q:1003:AMP:O5'	4:Q:1003:AMP:H8	2.03	0.42
1:Q:148:LYS:HE3	1:Q:148:LYS:HB3	1.31	0.42
1:C:197:ASP:HA	1:C:198:PRO:HD3	1.83	0.41
1:E:197:ASP:HB3	1:E:202:ALA:CB	2.49	0.41
1:E:290:TRP:CZ3	1:E:299:VAL:HG21	2.55	0.41
1:F:228:ILE:H	1:F:228:ILE:HG12	1.59	0.41
1:G:101:GLU:O	1:G:105:MSE:HE3	2.20	0.41
1:G:65:TYR:O	1:G:70:ILE:HB	2.20	0.41
1:H:249:SER:OG	1:H:251:GLN:CG	2.68	0.41
1:M:249:SER:OG	1:M:251:GLN:HG3	2.21	0.41
1:M:290:TRP:C	1:M:292:GLU:H	2.23	0.41
1:P:245:TYR:HA	1:P:272:LEU:HD11	1.98	0.41
1:R:228:ILE:CG2	1:R:260:TYR:O	2.68	0.41
1:A:189:PRO:HB3	1:A:237:GLY:HA2	2.01	0.41
1:A:205:THR:CG2	1:A:206:LEU:N	2.82	0.41
1:C:211:LYS:CE	1:C:215:LYS:HD2	2.51	0.41
4:D:1003:AMP:H2'	4:D:1003:AMP:O2P	2.20	0.41
1:E:286:ARG:O	1:E:289:HIS:N	2.53	0.41
1:E:29:LEU:HA	1:E:29:LEU:HD23	1.86	0.41
1:F:319:GLU:HB3	1:F:324:LEU:HB2	2.02	0.41
1:J:165:TYR:HB3	1:J:321:ALA:HB1	2.02	0.41
1:J:281:ARG:N	1:J:282:PRO:HD2	2.34	0.41
1:L:278:GLU:HA	1:L:278:GLU:OE1	2.19	0.41
1:M:141:VAL:O	1:M:174:ALA:CA	2.64	0.41
1:P:94:GLN:CA	1:P:97:VAL:HG12	2.49	0.41
1:B:200:PRO:O	1:B:216:LYS:HE2	2.20	0.41
1:B:86:HIS:HD2	1:B:132:ASP:HA	1.84	0.41
1:E:218:LYS:HB2	1:E:218:LYS:HE3	1.83	0.41
1:F:105:MSE:CA	1:F:105:MSE:CE	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:PRO:HB2	1:F:127:PRO:HD3	2.02	0.41
1:F:134:LEU:CB	1:F:169:PHE:CE1	2.97	0.41
1:H:126:PRO:CB	1:H:127:PRO:CD	2.96	0.41
1:J:177:PRO:C	1:J:178:LYS:CG	2.88	0.41
1:K:322:MSE:HE2	1:K:322:MSE:HB3	1.88	0.41
1:L:182:ARG:O	1:L:184:MSE:HE2	2.20	0.41
1:M:130:ALA:CB	1:M:154:THR:HB	2.50	0.41
1:M:64:LEU:CD2	1:M:287:TYR:CE1	3.02	0.41
1:N:55:ARG:HH21	1:Q:320:GLN:NE2	2.18	0.41
1:P:192:LYS:HZ3	4:P:1003:AMP:H5'1	1.85	0.41
1:P:105:MSE:HE1	1:P:149:GLN:O	2.19	0.41
1:P:125:TYR:N	1:P:126:PRO:HD3	2.29	0.41
1:Q:241:LEU:HB3	1:Q:268:PHE:HE2	1.85	0.41
1:Q:93:LEU:HD23	1:Q:96:ILE:HD13	2.02	0.41
1:N:118:VAL:HB	1:Q:99:ILE:HG13	2.01	0.41
1:R:251:GLN:HB3	1:R:256:LEU:HD12	2.01	0.41
1:R:96:ILE:O	1:R:160:ARG:NH1	2.51	0.41
1:D:86:HIS:CE1	1:D:136:TYR:OH	2.74	0.41
1:D:28:GLU:HG2	1:D:28:GLU:H	1.79	0.41
1:H:29:LEU:HD11	1:H:177:PRO:HB2	1.99	0.41
1:I:147:GLN:OE1	1:I:150:HIS:HD2	2.03	0.41
1:J:192:LYS:HE3	1:J:192:LYS:HB3	1.33	0.41
1:J:59:ARG:HH11	1:J:59:ARG:HG3	1.85	0.41
1:J:86:HIS:HE1	1:J:136:TYR:OH	2.04	0.41
1:K:187:VAL:HG13	1:K:202:ALA:HA	2.02	0.41
1:K:78:PHE:N	1:K:78:PHE:CD1	2.88	0.41
1:L:119:SER:O	1:L:122:LEU:HB2	2.21	0.41
1:M:306:LYS:O	1:M:310:VAL:HG23	2.21	0.41
1:N:152:GLU:HA	1:N:152:GLU:OE1	2.20	0.41
1:O:313:GLU:OE2	1:O:317:LYS:HE3	2.21	0.41
1:P:216:LYS:O	1:P:216:LYS:HG3	2.21	0.41
1:R:282:PRO:HB2	1:R:286:ARG:HH21	1.85	0.41
1:D:123:LEU:HD23	1:D:124:THR:HG23	2.02	0.41
1:D:165:TYR:CD2	1:D:321:ALA:O	2.74	0.41
1:E:184:MSE:HA	1:E:192:LYS:HA	2.03	0.41
1:E:85:ALA:O	1:E:135:LEU:HD11	2.20	0.41
1:H:192:LYS:O	1:H:193:MSE:C	2.59	0.41
1:I:289:HIS:O	1:I:293:SER:HB2	2.21	0.41
1:J:34:ASN:HA	1:J:34:ASN:HD22	1.77	0.41
1:L:27:VAL:CG1	1:L:27:VAL:O	2.69	0.41
1:I:326:ARG:NH2	1:L:301:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:GLN:CD	1:M:60:ARG:NH2	2.74	0.41
1:M:55:ARG:NH2	1:P:320:GLN:HA	2.36	0.41
1:P:76:THR:HG23	1:P:306:LYS:HE3	2.03	0.41
1:R:213:ILE:HG21	1:R:277:ILE:HG13	2.02	0.41
1:A:122:LEU:HD13	1:A:122:LEU:HA	1.79	0.41
1:C:230:TYR:CD1	1:C:239:SER:HB3	2.55	0.41
1:E:83:VAL:HG13	1:E:308:ASN:ND2	2.36	0.41
1:L:175:ARG:O	1:L:175:ARG:HG2	2.18	0.41
1:L:199:ASN:ND2	1:L:200:PRO:HD2	2.31	0.41
1:L:205:THR:O	1:L:208:ASP:HB2	2.21	0.41
1:P:213:ILE:O	1:P:217:ILE:HG13	2.21	0.41
1:B:129:MSE:HG3	2:B:1001:TRP:NE1	2.36	0.41
1:D:171:ILE:N	1:D:171:ILE:CD1	2.83	0.41
1:D:209:ASP:O	1:D:209:ASP:OD1	2.39	0.41
1:H:192:LYS:O	1:H:194:SER:N	2.53	0.41
1:J:295:GLU:O	1:J:299:VAL:HG23	2.20	0.41
1:K:258:ARG:C	1:K:261:GLU:HG3	2.37	0.41
1:L:129:MSE:O	1:L:132:ASP:HB2	2.21	0.41
1:N:168:LEU:HD22	1:N:314:MSE:SE	2.71	0.41
3:O:1002:PO4:O3	4:O:1003:AMP:O1P	2.39	0.41
1:O:71:ASP:HA	1:O:72:PRO:HD2	1.81	0.41
1:P:169:PHE:HE1	1:P:314:MSE:HE3	1.84	0.41
1:Q:205:THR:CG2	1:Q:206:LEU:N	2.83	0.41
1:Q:313:GLU:OE1	1:Q:313:GLU:HA	2.20	0.41
1:R:289:HIS:O	1:R:293:SER:N	2.53	0.41
1:D:209:ASP:OD1	1:D:209:ASP:C	2.59	0.41
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.21	0.41
1:F:160:ARG:HB2	1:F:160:ARG:HE	1.72	0.41
1:H:15:THR:CB	1:H:204:ILE:O	2.63	0.41
1:H:238:ILE:HD13	1:H:238:ILE:HA	1.92	0.41
1:J:59:ARG:CG	1:J:59:ARG:NH1	2.80	0.41
1:L:141:VAL:N	1:L:173:GLU:O	2.48	0.41
1:L:29:LEU:CD1	1:L:177:PRO:HG2	2.50	0.41
1:N:176:ILE:CG2	1:N:179:VAL:HG13	2.51	0.41
1:P:99:ILE:O	1:P:103:GLU:HG3	2.20	0.41
1:P:205:THR:HG22	1:P:207:LEU:N	2.25	0.41
1:P:217:ILE:CD1	1:P:273:ALA:HA	2.50	0.41
1:B:175:ARG:C	1:B:176:ILE:CG1	2.89	0.41
1:C:145:GLU:O	1:C:148:LYS:HB3	2.21	0.41
1:C:23:LEU:HG	1:C:68:VAL:HG11	2.02	0.41
1:E:238:ILE:O	1:E:239:SER:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ARG:CG	1:G:184:MSE:HE1	2.41	0.41
1:J:243:ASN:O	1:J:247:THR:HG23	2.21	0.41
1:K:190:THR:O	1:K:190:THR:HG22	2.21	0.41
1:M:241:LEU:HA	1:M:241:LEU:HD12	1.88	0.41
1:M:293:SER:OG	1:M:295:GLU:N	2.54	0.41
1:N:25:GLN:HG2	1:N:178:LYS:HB2	2.01	0.41
1:P:19:TYR:HA	1:P:23:LEU:HB3	2.02	0.41
1:P:245:TYR:O	1:P:249:SER:OG	2.37	0.41
1:Q:122:LEU:HA	1:Q:122:LEU:HD13	1.84	0.41
1:Q:242:LEU:O	1:Q:246:SER:HB3	2.21	0.41
1:Q:40:VAL:HG11	2:Q:1001:TRP:CD1	2.55	0.41
1:Q:30:GLN:O	1:Q:74:GLN:HG3	2.20	0.41
1:R:188:ASP:OD2	1:R:190:THR:HB	2.21	0.41
1:C:99:ILE:HG13	1:F:118:VAL:HB	2.03	0.41
1:D:53:GLU:OE1	1:D:53:GLU:HA	2.21	0.41
1:E:191:LYS:HG2	1:E:192:LYS:N	2.36	0.41
1:F:71:ASP:HA	1:F:72:PRO:HD2	1.86	0.41
4:H:1003:AMP:H4'	4:H:1003:AMP:O1P	2.21	0.41
1:J:205:THR:C	1:J:207:LEU:N	2.74	0.41
1:J:94:GLN:HA	1:J:97:VAL:HG12	2.02	0.41
1:L:281:ARG:CG	1:L:281:ARG:NH1	2.78	0.41
1:M:128:LEU:O	1:M:128:LEU:HD12	2.21	0.41
1:N:125:TYR:N	1:N:126:PRO:HD2	2.36	0.41
1:N:146:ASP:OD1	1:N:146:ASP:N	2.36	0.41
1:Q:140:ILE:HD12	1:Q:175:ARG:HG2	2.01	0.41
1:R:209:ASP:O	1:R:212:THR:N	2.54	0.41
1:R:260:TYR:N	1:R:260:TYR:CD2	2.89	0.41
1:A:150:HIS:O	1:A:154:THR:CG2	2.69	0.41
1:A:67:ALA:HB2	1:A:287:TYR:HA	2.03	0.41
1:D:212:THR:CG2	1:D:216:LYS:HD2	2.39	0.41
1:F:293:SER:OG	1:F:295:GLU:HB2	2.21	0.41
1:H:300:LEU:HD23	1:H:300:LEU:HA	1.95	0.41
1:I:106:THR:O	1:I:107:GLN:C	2.59	0.41
1:I:194:SER:HB2	3:I:1002:PO4:O2	2.21	0.41
1:N:245:TYR:CD2	1:N:256:LEU:CD2	3.04	0.41
1:O:193:MSE:CA	4:O:1003:AMP:N6	2.83	0.41
1:O:320:GLN:OE1	1:R:55:ARG:NH2	2.54	0.41
1:P:245:TYR:CG	1:P:272:LEU:HD13	2.51	0.41
1:P:279:THR:O	1:P:282:PRO:CD	2.64	0.41
1:Q:98:TYR:HB2	1:Q:101:GLU:HG3	2.03	0.41
1:R:146:ASP:N	1:R:146:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:137:ASN:ND2	1:R:170:THR:OG1	2.51	0.41
1:R:241:LEU:O	1:R:244:ILE:N	2.54	0.41
1:C:316:ARG:CG	1:C:316:ARG:NH2	2.77	0.40
1:E:71:ASP:HB3	1:E:74:GLN:CB	2.50	0.40
1:F:228:ILE:HD13	1:F:265:TYR:CD1	2.55	0.40
1:G:282:PRO:HB2	1:G:286:ARG:HH21	1.86	0.40
1:H:119:SER:HB2	1:K:95:CYS:O	2.21	0.40
1:I:29:LEU:CD1	1:I:177:PRO:HB2	2.51	0.40
1:J:65:TYR:O	1:J:70:ILE:HB	2.21	0.40
1:M:276:VAL:C	1:M:278:GLU:N	2.73	0.40
1:N:86:HIS:CD2	1:N:132:ASP:OD1	2.74	0.40
1:O:175:ARG:NH2	1:O:177:PRO:CG	2.84	0.40
1:P:122:LEU:O	1:P:125:TYR:CE1	2.74	0.40
1:P:230:TYR:CD1	1:P:230:TYR:C	2.94	0.40
1:Q:97:VAL:CG1	1:Q:97:VAL:O	2.69	0.40
1:A:199:ASN:ND2	1:A:201:LYS:HG3	2.36	0.40
1:A:228:ILE:HG13	1:A:260:TYR:HB3	2.03	0.40
1:B:146:ASP:OD1	1:B:146:ASP:N	2.41	0.40
1:G:162:ASN:CG	1:G:167:GLU:HA	2.41	0.40
1:H:245:TYR:HD2	1:H:268:PHE:CE1	2.39	0.40
1:I:29:LEU:O	1:I:33:TYR:HB2	2.21	0.40
1:N:19:TYR:HE1	1:N:68:VAL:HG13	1.86	0.40
1:O:195:LYS:HG3	1:O:196:SER:N	2.36	0.40
1:O:246:SER:HB2	1:O:251:GLN:O	2.21	0.40
1:O:213:ILE:CD1	1:O:280:LEU:HD12	2.51	0.40
1:O:59:ARG:CG	1:O:60:ARG:N	2.83	0.40
1:P:248:LEU:CD1	1:P:248:LEU:H	2.29	0.40
1:Q:229:ARG:HE	1:Q:229:ARG:HB3	1.38	0.40
1:Q:41:ASP:N	1:Q:41:ASP:OD1	2.55	0.40
1:R:21:GLY:HA3	4:R:1003:AMP:N3	2.36	0.40
1:A:123:LEU:HG	1:A:123:LEU:O	2.20	0.40
1:B:38:CYS:SG	1:B:80:GLN:CB	3.09	0.40
1:E:105:MSE:HA	1:E:105:MSE:CE	2.47	0.40
1:F:207:LEU:HD11	1:F:287:TYR:CZ	2.57	0.40
1:F:242:LEU:O	1:F:246:SER:HB3	2.22	0.40
1:G:224:SER:HB2	1:I:166:GLY:H	1.83	0.40
1:J:50:ASP:OD2	1:J:51:PRO:HD2	2.21	0.40
1:K:126:PRO:HD2	1:K:127:PRO:HD2	2.03	0.40
1:M:105:MSE:O	1:M:106:THR:C	2.59	0.40
1:M:126:PRO:CB	1:M:127:PRO:CD	2.96	0.40
1:M:199:ASN:HD22	1:M:200:PRO:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:ILE:HG12	1:N:140:ILE:HB	2.04	0.40
1:O:242:LEU:HA	1:O:242:LEU:HD23	1.91	0.40
1:O:24:ARG:HH11	1:O:24:ARG:CB	2.35	0.40
1:Q:140:ILE:HD13	1:Q:175:ARG:CZ	2.52	0.40
1:Q:197:ASP:HA	1:Q:198:PRO:HD3	1.89	0.40
1:R:64:LEU:O	1:R:67:ALA:HB3	2.21	0.40
1:A:151:ILE:HA	1:A:154:THR:HG23	2.03	0.40
1:A:70:ILE:HD13	1:A:70:ILE:HA	1.87	0.40
1:C:16:ILE:HA	1:C:19:TYR:CB	2.52	0.40
1:E:281:ARG:N	1:E:282:PRO:CD	2.84	0.40
1:E:30:GLN:HG3	1:E:74:GLN:HG3	1.96	0.40
1:E:78:PHE:CD1	1:E:78:PHE:N	2.89	0.40
1:G:130:ALA:HB2	1:G:154:THR:HB	2.02	0.40
1:H:40:VAL:HG23	1:H:40:VAL:O	2.21	0.40
1:I:86:HIS:HE1	1:I:136:TYR:OH	2.04	0.40
1:K:302:GLU:O	1:K:306:LYS:HG3	2.21	0.40
1:N:125:TYR:CD2	1:N:126:PRO:HD3	2.57	0.40
1:N:150:HIS:O	1:N:154:THR:CG2	2.68	0.40
1:N:43:HIS:O	1:N:46:THR:OG1	2.31	0.40
1:O:252:SER:OG	1:O:255:GLU:HB3	2.22	0.40
1:Q:168:LEU:HA	1:Q:168:LEU:HD23	1.91	0.40
1:Q:176:ILE:HA	1:Q:177:PRO:HD3	1.89	0.40
1:R:184:MSE:HB3	1:R:184:MSE:HE2	1.61	0.40
1:R:59:ARG:HH22	1:R:297:ASP:CG	2.23	0.40
1:B:252:SER:OG	1:B:255:GLU:HB2	2.22	0.40
1:G:104:ARG:HH11	1:G:104:ARG:HD3	1.77	0.40
1:J:185:SER:O	1:J:188:ASP:O	2.39	0.40
1:K:242:LEU:HD23	1:K:242:LEU:HA	1.87	0.40
1:K:41:ASP:N	1:K:41:ASP:OD1	2.55	0.40
1:P:184:MSE:N	1:P:240:ASN:HD21	2.19	0.40
1:Q:4:ILE:HD13	1:Q:140:ILE:CG2	2.52	0.40
1:R:25:GLN:N	1:R:25:GLN:CD	2.71	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/326 (87%)	273 (96%)	11 (4%)	1 (0%)	38	66
1	B	281/326 (86%)	266 (95%)	14 (5%)	1 (0%)	38	66
1	C	285/326 (87%)	273 (96%)	12 (4%)	0	100	100
1	D	291/326 (89%)	282 (97%)	9 (3%)	0	100	100
1	E	281/326 (86%)	252 (90%)	29 (10%)	0	100	100
1	F	284/326 (87%)	276 (97%)	8 (3%)	0	100	100
1	G	292/326 (90%)	272 (93%)	20 (7%)	0	100	100
1	H	291/326 (89%)	278 (96%)	12 (4%)	1 (0%)	44	73
1	I	288/326 (88%)	279 (97%)	9 (3%)	0	100	100
1	J	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	K	284/326 (87%)	269 (95%)	15 (5%)	0	100	100
1	L	291/326 (89%)	283 (97%)	8 (3%)	0	100	100
1	M	291/326 (89%)	269 (92%)	19 (6%)	3 (1%)	18	43
1	N	291/326 (89%)	281 (97%)	10 (3%)	0	100	100
1	O	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	P	283/326 (87%)	256 (90%)	27 (10%)	0	100	100
1	Q	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	R	276/326 (85%)	260 (94%)	16 (6%)	0	100	100
All	All	5167/5868 (88%)	4900 (95%)	261 (5%)	6 (0%)	55	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	GLY
1	H	193	MSE
1	M	291	MSE
1	A	246	SER
1	M	105	MSE
1	M	277	ILE

### 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	257/268 (96%)	219 (85%)	38 (15%)	3	9
1	B	256/268 (96%)	202 (79%)	54 (21%)	1	3
1	C	257/268 (96%)	211 (82%)	46 (18%)	2	5
1	D	259/268 (97%)	216 (83%)	43 (17%)	2	6
1	E	253/268 (94%)	208 (82%)	45 (18%)	2	5
1	F	255/268 (95%)	203 (80%)	52 (20%)	1	4
1	G	260/268 (97%)	219 (84%)	41 (16%)	3	7
1	H	259/268 (97%)	214 (83%)	45 (17%)	2	5
1	I	256/268 (96%)	203 (79%)	53 (21%)	1	3
1	J	259/268 (97%)	207 (80%)	52 (20%)	1	4
1	K	254/268 (95%)	210 (83%)	44 (17%)	2	6
1	L	259/268 (97%)	219 (85%)	40 (15%)	3	8
1	M	259/268 (97%)	202 (78%)	57 (22%)	1	3
1	N	259/268 (97%)	221 (85%)	38 (15%)	3	9
1	O	259/268 (97%)	194 (75%)	65 (25%)	0	2
1	P	255/268 (95%)	200 (78%)	55 (22%)	1	3
1	Q	259/268 (97%)	199 (77%)	60 (23%)	1	2
1	R	252/268 (94%)	196 (78%)	56 (22%)	1	3
All	All	4627/4824 (96%)	3743 (81%)	884 (19%)	2	4

All (884) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	8	ILE
1	A	9	GLN
1	A	25	GLN
1	A	28	GLU
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	60	ARG
1	A	73	THR
1	A	99	ILE
1	A	104	ARG
1	A	105	MSE
1	A	119	SER
1	A	122	LEU
1	A	138	THR
1	A	146	ASP
1	A	148	LYS
1	A	154	THR
1	A	164	ARG
1	A	173	GLU
1	A	175	ARG
1	A	182	ARG
1	A	197	ASP
1	A	199	ASN
1	A	201	LYS
1	A	205	THR
1	A	219	SER
1	A	228	ILE
1	A	238	ILE
1	A	241	LEU
1	A	245	TYR
1	A	247	THR
1	A	275	VAL
1	A	292	GLU
1	A	308	ASN
1	A	312	SER
1	A	317	LYS
1	A	320	GLN
1	B	2	LYS
1	B	24	ARG
1	B	32	GLU
1	B	55	ARG
1	B	59	ARG
1	B	70	ILE
1	B	73	THR
1	B	80	GLN
1	B	81	SER
1	B	96	ILE

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Mol	Chain	Res	Type
1	B	99	ILE
1	B	106	THR
1	B	119	SER
1	B	122	LEU
1	B	138	THR
1	B	145	GLU
1	B	146	ASP
1	B	154	THR
1	B	159	GLU
1	B	164	ARG
1	B	165	TYR
1	B	170	THR
1	B	171	ILE
1	B	175	ARG
1	B	185	SER
1	B	190	THR
1	B	192	LYS
1	B	195	LYS
1	B	199	ASN
1	B	205	THR
1	B	206	LEU
1	B	219	SER
1	B	225	GLU
1	B	227	THR
1	B	228	ILE
1	B	229	ARG
1	B	238	ILE
1	B	241	LEU
1	B	245	TYR
1	B	246	SER
1	B	247	THR
1	B	254	GLU
1	B	255	GLU
1	B	261	GLU
1	B	267	VAL
1	B	278	GLU
1	B	284	GLN
1	B	285	GLU
1	B	286	ARG
1	B	289	HIS
1	B	292	GLU
1	B	308	ASN

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Mol	Chain	Res	Type
1	B	312	SER
1	B	316	ARG
1	C	1	MSE
1	C	8	ILE
1	C	23	LEU
1	C	24	ARG
1	C	53	GLU
1	C	55	ARG
1	C	56	GLN
1	C	59	ARG
1	C	70	ILE
1	C	96	ILE
1	C	99	ILE
1	C	107	GLN
1	C	119	SER
1	C	122	LEU
1	C	138	THR
1	C	145	GLU
1	C	146	ASP
1	C	148	LYS
1	C	154	THR
1	C	164	ARG
1	C	168	LEU
1	C	175	ARG
1	C	182	ARG
1	C	185	SER
1	C	196	SER
1	C	199	ASN
1	C	201	LYS
1	C	217	ILE
1	C	219	SER
1	C	224	SER
1	C	238	ILE
1	C	241	LEU
1	C	245	TYR
1	C	246	SER
1	C	252	SER
1	C	253	ILE
1	C	267	VAL
1	C	275	VAL
1	C	278	GLU
1	C	281	ARG

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Mol	Chain	Res	Type
1	C	285	GLU
1	C	302	GLU
1	C	305	GLU
1	C	308	ASN
1	C	312	SER
1	C	316	ARG
1	D	1	MSE
1	D	8	ILE
1	D	9	GLN
1	D	28	GLU
1	D	29	LEU
1	D	55	ARG
1	D	56	GLN
1	D	59	ARG
1	D	96	ILE
1	D	99	ILE
1	D	107	GLN
1	D	122	LEU
1	D	137	ASN
1	D	138	THR
1	D	146	ASP
1	D	148	LYS
1	D	154	THR
1	D	159	GLU
1	D	160	ARG
1	D	164	ARG
1	D	185	SER
1	D	199	ASN
1	D	205	THR
1	D	211	LYS
1	D	219	SER
1	D	224	SER
1	D	225	GLU
1	D	229	ARG
1	D	241	LEU
1	D	245	TYR
1	D	247	THR
1	D	255	GLU
1	D	278	GLU
1	D	281	ARG
1	D	285	GLU
1	D	294	GLU

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Mol	Chain	Res	Type
1	D	302	GLU
1	D	308	ASN
1	D	309	ARG
1	D	312	SER
1	D	314	MSE
1	D	316	ARG
1	D	317	LYS
1	E	6	SER
1	E	20	ILE
1	E	23	LEU
1	E	25	GLN
1	E	27	VAL
1	E	32	GLU
1	E	53	GLU
1	E	55	ARG
1	E	56	GLN
1	E	96	ILE
1	E	104	ARG
1	E	105	MSE
1	E	106	THR
1	E	107	GLN
1	E	122	LEU
1	E	124	THR
1	E	138	THR
1	E	148	LYS
1	E	154	THR
1	E	160	ARG
1	E	173	GLU
1	E	175	ARG
1	E	178	LYS
1	E	201	LYS
1	E	206	LEU
1	E	211	LYS
1	E	215	LYS
1	E	218	LYS
1	E	225	GLU
1	E	238	ILE
1	E	239	SER
1	E	241	LEU
1	E	245	TYR
1	E	247	THR
1	E	248	LEU

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Mol	Chain	Res	Type
1	E	253	ILE
1	E	258	ARG
1	E	284	GLN
1	E	285	GLU
1	E	295	GLU
1	E	299	VAL
1	E	308	ASN
1	E	309	ARG
1	E	312	SER
1	E	320	GLN
1	F	1	MSE
1	F	8	ILE
1	F	18	ASN
1	F	24	ARG
1	F	32	GLU
1	F	34	ASN
1	F	55	ARG
1	F	56	GLN
1	F	59	ARG
1	F	60	ARG
1	F	73	THR
1	F	96	ILE
1	F	99	ILE
1	F	105	MSE
1	F	107	GLN
1	F	119	SER
1	F	122	LEU
1	F	123	LEU
1	F	138	THR
1	F	146	ASP
1	F	151	ILE
1	F	154	THR
1	F	160	ARG
1	F	164	ARG
1	F	175	ARG
1	F	182	ARG
1	F	188	ASP
1	F	190	THR
1	F	192	LYS
1	F	199	ASN
1	F	205	THR
1	F	211	LYS

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Mol	Chain	Res	Type
1	F	217	ILE
1	F	218	LYS
1	F	219	SER
1	F	225	GLU
1	F	227	THR
1	F	228	ILE
1	F	229	ARG
1	F	238	ILE
1	F	241	LEU
1	F	242	LEU
1	F	245	TYR
1	F	247	THR
1	F	251	GLN
1	F	254	GLU
1	F	278	GLU
1	F	281	ARG
1	F	289	HIS
1	F	293	SER
1	F	308	ASN
1	F	326	ARG
1	G	1	MSE
1	G	4	ILE
1	G	8	ILE
1	G	25	GLN
1	G	55	ARG
1	G	60	ARG
1	G	73	THR
1	G	74	GLN
1	G	78	PHE
1	G	81	SER
1	G	96	ILE
1	G	99	ILE
1	G	106	THR
1	G	107	GLN
1	G	122	LEU
1	G	138	THR
1	G	146	ASP
1	G	148	LYS
1	G	154	THR
1	G	164	ARG
1	G	171	ILE
1	G	182	ARG

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Mol	Chain	Res	Type
1	G	185	SER
1	G	199	ASN
1	G	205	THR
1	G	211	LYS
1	G	215	LYS
1	G	219	SER
1	G	229	ARG
1	G	241	LEU
1	G	245	TYR
1	G	254	GLU
1	G	263	LYS
1	G	277	ILE
1	G	278	GLU
1	G	285	GLU
1	G	298	ARG
1	G	308	ASN
1	G	309	ARG
1	G	320	GLN
1	G	326	ARG
1	H	8	ILE
1	H	9	GLN
1	H	53	GLU
1	H	55	ARG
1	H	56	GLN
1	H	59	ARG
1	H	76	THR
1	H	94	GLN
1	H	96	ILE
1	H	99	ILE
1	H	106	THR
1	H	119	SER
1	H	122	LEU
1	H	138	THR
1	H	148	LYS
1	H	154	THR
1	H	159	GLU
1	H	164	ARG
1	H	173	GLU
1	H	176	ILE
1	H	179	VAL
1	H	182	ARG
1	H	191	LYS

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Mol	Chain	Res	Type
1	H	192	LYS
1	H	194	SER
1	H	199	ASN
1	H	215	LYS
1	H	217	ILE
1	H	218	LYS
1	H	225	GLU
1	H	227	THR
1	H	228	ILE
1	H	241	LEU
1	H	245	TYR
1	H	251	GLN
1	H	267	VAL
1	H	274	GLN
1	H	293	SER
1	H	294	GLU
1	H	295	GLU
1	H	302	GLU
1	H	305	GLU
1	H	308	ASN
1	H	312	SER
1	H	316	ARG
1	I	1	MSE
1	I	8	ILE
1	I	9	GLN
1	I	16	ILE
1	I	24	ARG
1	I	25	GLN
1	I	26	PHE
1	I	28	GLU
1	I	50	ASP
1	I	53	GLU
1	I	55	ARG
1	I	56	GLN
1	I	59	ARG
1	I	60	ARG
1	I	70	ILE
1	I	81	SER
1	I	96	ILE
1	I	99	ILE
1	I	107	GLN
1	I	122	LEU

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Mol	Chain	Res	Type
1	I	138	THR
1	I	148	LYS
1	I	154	THR
1	I	160	ARG
1	I	164	ARG
1	I	176	ILE
1	I	178	LYS
1	I	179	VAL
1	I	182	ARG
1	I	191	LYS
1	I	192	LYS
1	I	194	SER
1	I	196	SER
1	I	199	ASN
1	I	211	LYS
1	I	215	LYS
1	I	219	SER
1	I	225	GLU
1	I	227	THR
1	I	238	ILE
1	I	241	LEU
1	I	245	TYR
1	I	252	SER
1	I	263	LYS
1	I	267	VAL
1	I	278	GLU
1	I	292	GLU
1	I	295	GLU
1	I	302	GLU
1	I	308	ASN
1	I	312	SER
1	I	314	MSE
1	I	320	GLN
1	J	1	MSE
1	J	8	ILE
1	J	9	GLN
1	J	23	LEU
1	J	24	ARG
1	J	28	GLU
1	J	55	ARG
1	J	56	GLN
1	J	59	ARG

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Mol	Chain	Res	Type
1	J	60	ARG
1	J	81	SER
1	J	94	GLN
1	J	96	ILE
1	J	99	ILE
1	J	104	ARG
1	J	105	MSE
1	J	106	THR
1	J	122	LEU
1	J	124	THR
1	J	138	THR
1	J	145	GLU
1	J	146	ASP
1	J	148	LYS
1	J	154	THR
1	J	159	GLU
1	J	160	ARG
1	J	164	ARG
1	J	175	ARG
1	J	178	LYS
1	J	179	VAL
1	J	190	THR
1	J	192	LYS
1	J	199	ASN
1	J	205	THR
1	J	215	LYS
1	J	219	SER
1	J	225	GLU
1	J	227	THR
1	J	229	ARG
1	J	238	ILE
1	J	239	SER
1	J	241	LEU
1	J	245	TYR
1	J	277	ILE
1	J	278	GLU
1	J	281	ARG
1	J	308	ASN
1	J	309	ARG
1	J	312	SER
1	J	315	VAL
1	J	320	GLN

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Mol	Chain	Res	Type
1	J	326	ARG
1	K	8	ILE
1	K	16	ILE
1	K	23	LEU
1	K	24	ARG
1	K	53	GLU
1	K	55	ARG
1	K	56	GLN
1	K	60	ARG
1	K	94	GLN
1	K	96	ILE
1	K	99	ILE
1	K	119	SER
1	K	122	LEU
1	K	138	THR
1	K	145	GLU
1	K	146	ASP
1	K	149	GLN
1	K	154	THR
1	K	164	ARG
1	K	175	ARG
1	K	179	VAL
1	K	182	ARG
1	K	187	VAL
1	K	191	LYS
1	K	192	LYS
1	K	195	LYS
1	K	196	SER
1	K	199	ASN
1	K	204	ILE
1	K	205	THR
1	K	206	LEU
1	K	211	LYS
1	K	215	LYS
1	K	218	LYS
1	K	219	SER
1	K	241	LEU
1	K	256	LEU
1	K	259	GLN
1	K	267	VAL
1	K	295	GLU
1	K	308	ASN

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Mol	Chain	Res	Type
1	K	312	SER
1	K	320	GLN
1	K	322	MSE
1	L	2	LYS
1	L	20	ILE
1	L	24	ARG
1	L	25	GLN
1	L	55	ARG
1	L	56	GLN
1	L	59	ARG
1	L	60	ARG
1	L	81	SER
1	L	96	ILE
1	L	99	ILE
1	L	119	SER
1	L	122	LEU
1	L	138	THR
1	L	145	GLU
1	L	146	ASP
1	L	154	THR
1	L	159	GLU
1	L	164	ARG
1	L	167	GLU
1	L	175	ARG
1	L	182	ARG
1	L	194	SER
1	L	199	ASN
1	L	205	THR
1	L	227	THR
1	L	228	ILE
1	L	238	ILE
1	L	241	LEU
1	L	245	TYR
1	L	246	SER
1	L	252	SER
1	L	285	GLU
1	L	289	HIS
1	L	293	SER
1	L	295	GLU
1	L	308	ASN
1	L	309	ARG
1	L	312	SER

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Mol	Chain	Res	Type
1	L	316	ARG
1	M	8	ILE
1	M	16	ILE
1	M	18	ASN
1	M	32	GLU
1	M	56	GLN
1	M	59	ARG
1	M	60	ARG
1	M	73	THR
1	M	74	GLN
1	M	94	GLN
1	M	96	ILE
1	M	99	ILE
1	M	107	GLN
1	M	119	SER
1	M	122	LEU
1	M	138	THR
1	M	140	ILE
1	M	146	ASP
1	M	148	LYS
1	M	151	ILE
1	M	154	THR
1	M	164	ARG
1	M	171	ILE
1	M	173	GLU
1	M	176	ILE
1	M	182	ARG
1	M	185	SER
1	M	187	VAL
1	M	190	THR
1	M	195	LYS
1	M	199	ASN
1	M	206	LEU
1	M	211	LYS
1	M	219	SER
1	M	227	THR
1	M	229	ARG
1	M	241	LEU
1	M	245	TYR
1	M	246	SER
1	M	251	GLN
1	M	253	ILE

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Mol	Chain	Res	Type
1	M	257	GLU
1	M	267	VAL
1	M	278	GLU
1	M	279	THR
1	M	281	ARG
1	M	289	HIS
1	M	292	GLU
1	M	293	SER
1	M	294	GLU
1	M	297	ASP
1	M	305	GLU
1	M	308	ASN
1	M	312	SER
1	M	316	ARG
1	M	320	GLN
1	M	326	ARG
1	N	1	MSE
1	N	8	ILE
1	N	24	ARG
1	N	53	GLU
1	N	55	ARG
1	N	59	ARG
1	N	96	ILE
1	N	99	ILE
1	N	107	GLN
1	N	122	LEU
1	N	129	MSE
1	N	138	THR
1	N	145	GLU
1	N	146	ASP
1	N	149	GLN
1	N	154	THR
1	N	164	ARG
1	N	168	LEU
1	N	179	VAL
1	N	182	ARG
1	N	187	VAL
1	N	191	LYS
1	N	192	LYS
1	N	195	LYS
1	N	199	ASN
1	N	211	LYS

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Mol	Chain	Res	Type
1	N	215	LYS
1	N	217	ILE
1	N	219	SER
1	N	225	GLU
1	N	241	LEU
1	N	253	ILE
1	N	278	GLU
1	N	292	GLU
1	N	294	GLU
1	N	308	ASN
1	N	312	SER
1	N	316	ARG
1	O	1	MSE
1	O	4	ILE
1	O	8	ILE
1	O	18	ASN
1	O	23	LEU
1	O	24	ARG
1	O	25	GLN
1	O	28	GLU
1	O	31	HIS
1	O	32	GLU
1	O	34	ASN
1	O	55	ARG
1	O	56	GLN
1	O	59	ARG
1	O	70	ILE
1	O	81	SER
1	O	96	ILE
1	O	99	ILE
1	O	105	MSE
1	O	106	THR
1	O	107	GLN
1	O	119	SER
1	O	122	LEU
1	O	123	LEU
1	O	146	ASP
1	O	148	LYS
1	O	152	GLU
1	O	154	THR
1	O	159	GLU
1	O	160	ARG

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Mol	Chain	Res	Type
1	O	164	ARG
1	O	167	GLU
1	O	171	ILE
1	O	173	GLU
1	O	175	ARG
1	O	179	VAL
1	O	187	VAL
1	O	191	LYS
1	O	195	LYS
1	O	196	SER
1	O	199	ASN
1	O	205	THR
1	O	211	LYS
1	O	215	LYS
1	O	217	ILE
1	O	219	SER
1	O	225	GLU
1	O	227	THR
1	O	229	ARG
1	O	241	LEU
1	O	245	TYR
1	O	246	SER
1	O	247	THR
1	O	251	GLN
1	O	259	GLN
1	O	267	VAL
1	O	281	ARG
1	O	284	GLN
1	O	285	GLU
1	O	289	HIS
1	O	293	SER
1	O	297	ASP
1	O	305	GLU
1	O	308	ASN
1	O	316	ARG
1	P	1	MSE
1	P	8	ILE
1	P	9	GLN
1	P	16	ILE
1	P	18	ASN
1	P	24	ARG
1	P	28	GLU

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Mol	Chain	Res	Type
1	P	32	GLU
1	P	47	VAL
1	P	53	GLU
1	P	55	ARG
1	P	56	GLN
1	P	96	ILE
1	P	99	ILE
1	P	101	GLU
1	P	118	VAL
1	P	129	MSE
1	P	138	THR
1	P	146	ASP
1	P	154	THR
1	P	159	GLU
1	P	160	ARG
1	P	161	PHE
1	P	168	LEU
1	P	173	GLU
1	P	182	ARG
1	P	183	ILE
1	P	191	LYS
1	P	195	LYS
1	P	196	SER
1	P	199	ASN
1	P	201	LYS
1	P	205	THR
1	P	215	LYS
1	P	216	LYS
1	P	218	LYS
1	P	228	ILE
1	P	238	ILE
1	P	246	SER
1	P	248	LEU
1	P	252	SER
1	P	253	ILE
1	P	254	GLU
1	P	279	THR
1	P	280	LEU
1	P	281	ARG
1	P	284	GLN
1	P	285	GLU
1	P	292	GLU

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Mol	Chain	Res	Type
1	P	296	LEU
1	P	302	GLU
1	P	308	ASN
1	P	312	SER
1	P	320	GLN
1	P	326	ARG
1	Q	1	MSE
1	Q	4	ILE
1	Q	8	ILE
1	Q	9	GLN
1	Q	18	ASN
1	Q	24	ARG
1	Q	25	GLN
1	Q	30	GLN
1	Q	32	GLU
1	Q	53	GLU
1	Q	55	ARG
1	Q	56	GLN
1	Q	59	ARG
1	Q	60	ARG
1	Q	68	VAL
1	Q	96	ILE
1	Q	97	VAL
1	Q	99	ILE
1	Q	105	MSE
1	Q	118	VAL
1	Q	119	SER
1	Q	122	LEU
1	Q	138	THR
1	Q	146	ASP
1	Q	148	LYS
1	Q	154	THR
1	Q	155	ARG
1	Q	159	GLU
1	Q	164	ARG
1	Q	167	GLU
1	Q	168	LEU
1	Q	173	GLU
1	Q	176	ILE
1	Q	179	VAL
1	Q	185	SER
1	Q	188	ASP

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Mol	Chain	Res	Type
1	Q	190	THR
1	Q	192	LYS
1	Q	196	SER
1	Q	199	ASN
1	Q	205	THR
1	Q	217	ILE
1	Q	224	SER
1	Q	228	ILE
1	Q	229	ARG
1	Q	241	LEU
1	Q	245	TYR
1	Q	246	SER
1	Q	252	SER
1	Q	261	GLU
1	Q	267	VAL
1	Q	274	GLN
1	Q	277	ILE
1	Q	278	GLU
1	Q	295	GLU
1	Q	302	GLU
1	Q	308	ASN
1	Q	312	SER
1	Q	320	GLN
1	Q	326	ARG
1	R	1	MSE
1	R	4	ILE
1	R	8	ILE
1	R	9	GLN
1	R	15	THR
1	R	18	ASN
1	R	23	LEU
1	R	32	GLU
1	R	55	ARG
1	R	56	GLN
1	R	59	ARG
1	R	60	ARG
1	R	76	THR
1	R	96	ILE
1	R	99	ILE
1	R	101	GLU
1	R	106	THR
1	R	119	SER

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Mol	Chain	Res	Type
1	R	122	LEU
1	R	138	THR
1	R	146	ASP
1	R	148	LYS
1	R	154	THR
1	R	159	GLU
1	R	160	ARG
1	R	161	PHE
1	R	164	ARG
1	R	167	GLU
1	R	168	LEU
1	R	171	ILE
1	R	176	ILE
1	R	182	ARG
1	R	184	MSE
1	R	187	VAL
1	R	191	LYS
1	R	197	ASP
1	R	204	ILE
1	R	212	THR
1	R	214	GLU
1	R	215	LYS
1	R	216	LYS
1	R	219	SER
1	R	225	GLU
1	R	241	LEU
1	R	245	TYR
1	R	248	LEU
1	R	272	LEU
1	R	275	VAL
1	R	278	GLU
1	R	284	GLN
1	R	286	ARG
1	R	292	GLU
1	R	295	GLU
1	R	297	ASP
1	R	298	ARG
1	R	312	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
1	A	25	GLN
1	A	34	ASN
1	A	43	HIS
1	A	52	HIS
1	A	86	HIS
1	A	94	GLN
1	A	150	HIS
1	A	199	ASN
1	A	284	GLN
1	A	308	ASN
1	A	320	GLN
1	B	18	ASN
1	B	25	GLN
1	B	34	ASN
1	B	43	HIS
1	B	86	HIS
1	B	94	GLN
1	B	107	GLN
1	B	137	ASN
1	B	199	ASN
1	B	284	GLN
1	B	308	ASN
1	B	320	GLN
1	C	9	GLN
1	C	31	HIS
1	C	34	ASN
1	C	43	HIS
1	C	86	HIS
1	C	137	ASN
1	C	150	HIS
1	C	199	ASN
1	C	284	GLN
1	C	308	ASN
1	C	320	GLN
1	D	18	ASN
1	D	34	ASN
1	D	43	HIS
1	D	86	HIS
1	D	94	GLN
1	D	107	GLN
1	D	150	HIS

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Mol	Chain	Res	Type
1	D	199	ASN
1	D	284	GLN
1	D	320	GLN
1	E	9	GLN
1	E	34	ASN
1	E	86	HIS
1	E	288	HIS
1	E	308	ASN
1	E	320	GLN
1	F	18	ASN
1	F	34	ASN
1	F	43	HIS
1	F	86	HIS
1	F	107	GLN
1	F	137	ASN
1	F	150	HIS
1	F	199	ASN
1	F	308	ASN
1	F	320	GLN
1	G	18	ASN
1	G	25	GLN
1	G	34	ASN
1	G	43	HIS
1	G	86	HIS
1	G	107	GLN
1	G	150	HIS
1	G	199	ASN
1	G	259	GLN
1	G	308	ASN
1	G	320	GLN
1	H	9	GLN
1	H	31	HIS
1	H	34	ASN
1	H	43	HIS
1	H	52	HIS
1	H	56	GLN
1	H	86	HIS
1	H	137	ASN
1	H	150	HIS
1	H	199	ASN
1	H	308	ASN
1	H	320	GLN

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Mol	Chain	Res	Type
1	I	9	GLN
1	I	18	ASN
1	I	34	ASN
1	I	43	HIS
1	I	86	HIS
1	I	107	GLN
1	I	150	HIS
1	I	199	ASN
1	I	259	GLN
1	I	284	GLN
1	J	34	ASN
1	J	43	HIS
1	J	56	GLN
1	J	86	HIS
1	J	199	ASN
1	J	259	GLN
1	J	284	GLN
1	J	308	ASN
1	K	9	GLN
1	K	18	ASN
1	K	34	ASN
1	K	43	HIS
1	K	56	GLN
1	K	86	HIS
1	K	149	GLN
1	K	150	HIS
1	K	199	ASN
1	K	320	GLN
1	L	25	GLN
1	L	34	ASN
1	L	43	HIS
1	L	86	HIS
1	L	94	GLN
1	L	107	GLN
1	L	150	HIS
1	L	199	ASN
1	L	308	ASN
1	L	320	GLN
1	M	9	GLN
1	M	18	ASN
1	M	31	HIS
1	M	34	ASN

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Mol	Chain	Res	Type
1	M	56	GLN
1	M	74	GLN
1	M	86	HIS
1	M	94	GLN
1	M	137	ASN
1	M	199	ASN
1	M	259	GLN
1	M	284	GLN
1	M	288	HIS
1	M	308	ASN
1	M	320	GLN
1	N	9	GLN
1	N	34	ASN
1	N	43	HIS
1	N	52	HIS
1	N	86	HIS
1	N	94	GLN
1	N	107	GLN
1	N	150	HIS
1	N	199	ASN
1	N	251	GLN
1	N	259	GLN
1	N	284	GLN
1	O	9	GLN
1	O	34	ASN
1	O	86	HIS
1	O	107	GLN
1	O	150	HIS
1	O	199	ASN
1	O	259	GLN
1	P	9	GLN
1	P	34	ASN
1	P	86	HIS
1	P	150	HIS
1	P	199	ASN
1	P	240	ASN
1	P	308	ASN
1	P	320	GLN
1	Q	9	GLN
1	Q	25	GLN
1	Q	34	ASN
1	Q	43	HIS

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Mol	Chain	Res	Type
1	Q	86	HIS
1	Q	94	GLN
1	Q	107	GLN
1	Q	150	HIS
1	Q	199	ASN
1	Q	251	GLN
1	Q	259	GLN
1	Q	308	ASN
1	Q	320	GLN
1	R	18	ASN
1	R	34	ASN
1	R	43	HIS
1	R	57	ASN
1	R	74	GLN
1	R	80	GLN
1	R	86	HIS
1	R	107	GLN
1	R	137	ASN
1	R	149	GLN
1	R	150	HIS
1	R	240	ASN
1	R	308	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

54 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	TRP	A	1001	-	11,16,16	0.67	0	11,22,22	0.84	0
3	PO4	A	1002	-	4,4,4	2.08	1 (25%)	6,6,6	0.52	0
4	AMP	A	1003	-	22,25,25	1.26	2 (9%)	24,38,38	1.37	2 (8%)
2	TRP	B	1001	-	11,16,16	0.74	0	11,22,22	0.72	0
3	PO4	B	1002	-	4,4,4	2.11	1 (25%)	6,6,6	0.47	0
4	AMP	B	1003	-	22,25,25	1.06	2 (9%)	24,38,38	1.05	1 (4%)
2	TRP	C	1001	-	11,16,16	0.70	0	11,22,22	0.87	0
3	PO4	C	1002	-	4,4,4	2.12	1 (25%)	6,6,6	0.42	0
4	AMP	C	1003	-	22,25,25	1.10	2 (9%)	24,38,38	1.00	1 (4%)
2	TRP	D	1001	-	11,16,16	0.75	0	11,22,22	0.72	0
3	PO4	D	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.37	0
4	AMP	D	1003	-	22,25,25	1.06	2 (9%)	24,38,38	0.87	0
2	TRP	E	1001	-	11,16,16	0.71	0	11,22,22	0.83	0
3	PO4	E	1002	-	4,4,4	2.25	1 (25%)	6,6,6	0.48	0
4	AMP	E	1003	-	22,25,25	1.06	2 (9%)	24,38,38	1.02	1 (4%)
2	TRP	F	1001	-	11,16,16	0.73	0	11,22,22	0.76	0
3	PO4	F	1002	-	4,4,4	1.98	1 (25%)	6,6,6	0.42	0
4	AMP	F	1003	-	22,25,25	1.11	2 (9%)	24,38,38	0.86	0
2	TRP	G	1001	-	11,16,16	0.66	0	11,22,22	0.86	0
3	PO4	G	1002	-	4,4,4	2.10	1 (25%)	6,6,6	0.42	0
4	AMP	G	1003	-	22,25,25	1.10	2 (9%)	24,38,38	0.79	0
2	TRP	H	1001	-	11,16,16	0.71	0	11,22,22	0.78	0
3	PO4	H	1002	-	4,4,4	2.14	1 (25%)	6,6,6	0.42	0
4	AMP	H	1003	-	22,25,25	1.05	2 (9%)	24,38,38	2.39	4 (16%)
2	TRP	I	1001	-	11,16,16	0.70	0	11,22,22	0.86	0
3	PO4	I	1002	-	4,4,4	2.13	1 (25%)	6,6,6	0.33	0
4	AMP	I	1003	-	22,25,25	1.08	1 (4%)	24,38,38	1.32	3 (12%)
2	TRP	J	1001	-	11,16,16	0.70	0	11,22,22	0.88	0
3	PO4	J	1002	-	4,4,4	2.19	1 (25%)	6,6,6	0.65	0
4	AMP	J	1003	-	22,25,25	1.01	1 (4%)	24,38,38	0.91	0
2	TRP	K	1001	-	11,16,16	0.70	0	11,22,22	0.84	0
3	PO4	K	1002	-	4,4,4	1.99	1 (25%)	6,6,6	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	AMP	K	1003	-	22,25,25	0.98	1 (4%)	24,38,38	0.98	1 (4%)
2	TRP	L	1001	-	11,16,16	0.68	0	11,22,22	0.87	0
3	PO4	L	1002	-	4,4,4	2.13	1 (25%)	6,6,6	0.56	0
4	AMP	L	1003	-	22,25,25	1.03	2 (9%)	24,38,38	0.98	0
2	TRP	M	1001	-	11,16,16	0.69	0	11,22,22	0.86	0
3	PO4	M	1002	-	4,4,4	1.45	0	6,6,6	0.72	0
4	AMP	M	1003	-	22,25,25	0.84	1 (4%)	24,38,38	2.12	6 (25%)
2	TRP	N	1001	-	11,16,16	0.70	0	11,22,22	0.84	0
3	PO4	N	1002	-	4,4,4	2.09	1 (25%)	6,6,6	0.42	0
4	AMP	N	1003	-	22,25,25	1.32	3 (13%)	24,38,38	1.37	4 (16%)
2	TRP	O	1001	-	11,16,16	0.69	0	11,22,22	0.88	0
3	PO4	O	1002	-	4,4,4	2.08	1 (25%)	6,6,6	0.41	0
4	AMP	O	1003	-	22,25,25	1.10	2 (9%)	24,38,38	1.46	3 (12%)
2	TRP	P	1001	-	11,16,16	0.73	0	11,22,22	0.71	0
3	PO4	P	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.79	0
4	AMP	P	1003	-	22,25,25	0.91	1 (4%)	24,38,38	1.63	2 (8%)
2	TRP	Q	1001	-	11,16,16	0.69	0	11,22,22	0.86	0
3	PO4	Q	1002	-	4,4,4	2.08	1 (25%)	6,6,6	0.36	0
4	AMP	Q	1003	-	22,25,25	1.09	2 (9%)	24,38,38	1.00	1 (4%)
2	TRP	R	1001	-	11,16,16	0.70	0	11,22,22	0.86	0
3	PO4	R	1002	-	4,4,4	1.91	1 (25%)	6,6,6	0.38	0
4	AMP	R	1003	-	22,25,25	1.07	2 (9%)	24,38,38	0.85	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	TRP	A	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	A	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	B	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	B	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	C	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	C	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	D	1001	-	-	0/3/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	D	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	D	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	E	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	E	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	E	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	F	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	F	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	F	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	G	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	G	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	G	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	H	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	H	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	H	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	I	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	I	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	I	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	J	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	J	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	J	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	K	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	K	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	K	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	L	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	L	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	L	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	M	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	M	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	M	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	N	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	N	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	N	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	O	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	O	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	O	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	P	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	P	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	P	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	Q	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	Q	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	Q	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	R	1001	-	-	0/3/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	R	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	R	1003	-	-	0/6/26/26	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	AMP	C8-N7	-2.60	1.29	1.34
4	N	1003	AMP	C8-N7	-2.26	1.30	1.34
4	G	1003	AMP	C2-N3	2.02	1.35	1.32
4	C	1003	AMP	C2-N3	2.07	1.35	1.32
4	D	1003	AMP	C2-N3	2.07	1.35	1.32
4	B	1003	AMP	C2-N3	2.13	1.35	1.32
4	L	1003	AMP	C2-N3	2.15	1.35	1.32
4	F	1003	AMP	C2-N3	2.18	1.35	1.32
4	Q	1003	AMP	C2-N3	2.19	1.35	1.32
4	R	1003	AMP	C2-N3	2.20	1.35	1.32
4	N	1003	AMP	C2-N3	2.25	1.35	1.32
4	E	1003	AMP	C2-N3	2.31	1.36	1.32
4	M	1003	AMP	C5-C4	2.32	1.45	1.40
4	H	1003	AMP	C2-N3	2.34	1.36	1.32
4	P	1003	AMP	O4'-C1'	2.39	1.44	1.41
4	O	1003	AMP	C2-N3	2.57	1.36	1.32
4	H	1003	AMP	O4'-C1'	2.58	1.44	1.41
4	O	1003	AMP	O4'-C1'	3.03	1.45	1.41
4	E	1003	AMP	O4'-C1'	3.12	1.45	1.41
4	K	1003	AMP	O4'-C1'	3.21	1.45	1.41
3	R	1002	PO4	P-O1	3.38	1.57	1.50
3	K	1002	PO4	P-O1	3.46	1.57	1.50
4	L	1003	AMP	O4'-C1'	3.46	1.46	1.41
3	P	1002	PO4	P-O1	3.46	1.57	1.50
3	F	1002	PO4	P-O1	3.50	1.58	1.50
4	B	1003	AMP	O4'-C1'	3.50	1.46	1.41
4	R	1003	AMP	O4'-C1'	3.60	1.46	1.41
3	O	1002	PO4	P-O1	3.64	1.58	1.50
3	D	1002	PO4	P-O1	3.64	1.58	1.50
4	J	1003	AMP	O4'-C1'	3.65	1.46	1.41
3	A	1002	PO4	P-O1	3.66	1.58	1.50
3	Q	1002	PO4	P-O1	3.67	1.58	1.50
4	D	1003	AMP	O4'-C1'	3.67	1.46	1.41
3	N	1002	PO4	P-O1	3.68	1.58	1.50
3	J	1002	PO4	P-O1	3.73	1.58	1.50
3	G	1002	PO4	P-O1	3.74	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	PO4	P-O1	3.74	1.58	1.50
3	B	1002	PO4	P-O1	3.75	1.58	1.50
4	F	1003	AMP	O4'-C1'	3.75	1.46	1.41
3	H	1002	PO4	P-O1	3.75	1.58	1.50
3	L	1002	PO4	P-O1	3.75	1.58	1.50
4	C	1003	AMP	O4'-C1'	3.76	1.46	1.41
4	Q	1003	AMP	O4'-C1'	3.78	1.46	1.41
3	I	1002	PO4	P-O1	3.90	1.58	1.50
4	G	1003	AMP	O4'-C1'	3.90	1.46	1.41
3	E	1002	PO4	P-O1	3.91	1.58	1.50
4	I	1003	AMP	O4'-C1'	3.92	1.46	1.41
4	N	1003	AMP	O4'-C1'	4.17	1.47	1.41
4	A	1003	AMP	O4'-C1'	4.20	1.47	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	C4'-O4'-C1'	-9.96	99.17	109.77
4	M	1003	AMP	N3-C2-N1	-7.46	122.36	128.86
4	P	1003	AMP	C4'-O4'-C1'	-5.35	104.08	109.77
4	A	1003	AMP	P-O5'-C5'	-4.40	106.17	118.30
4	B	1003	AMP	C4'-O4'-C1'	-3.24	106.32	109.77
4	I	1003	AMP	P-O5'-C5'	-3.18	109.54	118.30
4	N	1003	AMP	C4'-O4'-C1'	-3.02	106.55	109.77
4	I	1003	AMP	C4'-O4'-C1'	-3.02	106.55	109.77
4	M	1003	AMP	C1'-N9-C4	-2.97	121.50	126.64
4	O	1003	AMP	N3-C2-N1	-2.85	126.38	128.86
4	E	1003	AMP	C4'-O4'-C1'	-2.82	106.77	109.77
4	C	1003	AMP	C4'-O4'-C1'	-2.77	106.82	109.77
4	N	1003	AMP	C2'-C3'-C4'	-2.60	97.55	102.62
4	M	1003	AMP	O3'-C3'-C2'	-2.48	103.89	111.83
4	K	1003	AMP	C4'-O4'-C1'	-2.46	107.15	109.77
4	Q	1003	AMP	C4'-O4'-C1'	-2.31	107.31	109.77
4	A	1003	AMP	O2'-C2'-C3'	-2.15	104.95	111.83
4	N	1003	AMP	C5'-C4'-C3'	-2.06	107.42	115.29
4	H	1003	AMP	C2'-C3'-C4'	-2.03	98.67	102.62
4	I	1003	AMP	O3P-P-O5'	2.01	112.07	106.73
4	H	1003	AMP	O4'-C4'-C5'	2.06	116.34	109.40
4	M	1003	AMP	C2-N1-C6	2.09	122.43	118.77
4	M	1003	AMP	O4'-C4'-C3'	2.11	109.37	105.17
4	O	1003	AMP	O4'-C4'-C3'	2.16	109.46	105.17
4	N	1003	AMP	C4-C5-N7	2.39	111.72	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1003	AMP	N6-C6-N1	2.65	124.02	118.77
4	H	1003	AMP	O5'-P-O1P	3.24	115.56	106.47
4	P	1003	AMP	O3P-P-O5'	4.20	117.91	106.73
4	O	1003	AMP	C4-C5-N7	4.49	113.75	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

37 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PO4	1	0
4	A	1003	AMP	10	0
2	B	1001	TRP	1	0
3	B	1002	PO4	1	0
4	B	1003	AMP	8	0
2	C	1001	TRP	2	0
4	C	1003	AMP	3	0
4	D	1003	AMP	5	0
3	E	1002	PO4	3	0
4	E	1003	AMP	4	0
3	F	1002	PO4	2	0
4	F	1003	AMP	2	0
2	G	1001	TRP	2	0
3	G	1002	PO4	1	0
4	G	1003	AMP	9	0
2	H	1001	TRP	1	0
3	H	1002	PO4	2	0
4	H	1003	AMP	1	0
3	I	1002	PO4	1	0
4	I	1003	AMP	7	0
2	J	1001	TRP	2	0
4	J	1003	AMP	3	0
3	K	1002	PO4	1	0
4	K	1003	AMP	4	0
4	L	1003	AMP	1	0
3	M	1002	PO4	3	0
4	M	1003	AMP	5	0
3	N	1002	PO4	2	0
4	N	1003	AMP	6	0
3	O	1002	PO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	1003	AMP	17	0
3	P	1002	PO4	7	0
4	P	1003	AMP	12	0
2	Q	1001	TRP	1	0
4	Q	1003	AMP	7	0
3	R	1002	PO4	1	0
4	R	1003	AMP	4	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	287/326 (88%)	0.20	14 (4%) 30 29	23, 45, 67, 89	0
1	B	285/326 (87%)	0.57	26 (9%) 10 7	41, 56, 80, 95	0
1	C	287/326 (88%)	0.28	9 (3%) 49 49	28, 43, 63, 86	0
1	D	291/326 (89%)	0.28	17 (5%) 24 22	29, 43, 66, 87	0
1	E	283/326 (86%)	0.82	44 (15%) 2 2	37, 63, 100, 125	0
1	F	286/326 (87%)	0.49	26 (9%) 10 7	32, 50, 73, 91	0
1	G	292/326 (89%)	0.42	25 (8%) 11 9	36, 51, 76, 92	0
1	H	291/326 (89%)	0.64	36 (12%) 4 4	26, 54, 79, 96	0
1	I	288/326 (88%)	0.27	14 (4%) 30 29	28, 44, 69, 89	0
1	J	291/326 (89%)	0.27	11 (3%) 41 39	31, 44, 67, 91	0
1	K	286/326 (87%)	0.73	32 (11%) 6 4	29, 58, 95, 120	0
1	L	291/326 (89%)	0.32	21 (7%) 16 14	24, 42, 68, 83	0
1	M	291/326 (89%)	1.21	72 (24%) 1 1	49, 69, 93, 106	0
1	N	291/326 (89%)	0.23	19 (6%) 20 17	25, 43, 65, 92	0
1	O	291/326 (89%)	0.81	43 (14%) 3 2	44, 60, 85, 98	0
1	P	285/326 (87%)	0.93	50 (17%) 2 1	44, 69, 110, 135	0
1	Q	291/326 (89%)	0.33	17 (5%) 24 22	28, 43, 68, 86	0
1	R	280/326 (85%)	1.06	58 (20%) 1 1	27, 67, 118, 137	0
All	All	5187/5868 (88%)	0.55	534 (10%) 7 5	23, 52, 88, 137	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	256	LEU	9.4
1	E	229	ARG	8.3
1	R	254	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	230	TYR	7.2
1	P	230	TYR	6.9
1	M	179	VAL	6.8
1	R	255	GLU	6.3
1	M	287	TYR	6.3
1	H	196	SER	6.2
1	E	256	LEU	6.1
1	R	259	GLN	6.1
1	P	226	GLY	6.0
1	R	252	SER	5.9
1	L	254	GLU	5.8
1	G	179	VAL	5.8
1	R	260	TYR	5.8
1	R	258	ARG	5.7
1	P	224	SER	5.7
1	M	288	HIS	5.6
1	E	226	GLY	5.5
1	H	106	THR	5.4
1	E	224	SER	5.4
1	R	224	SER	5.3
1	J	261	GLU	5.3
1	M	52	HIS	5.1
1	E	237	GLY	5.0
1	D	106	THR	5.0
1	M	212	THR	5.0
1	H	181	ALA	5.0
1	E	252	SER	5.0
1	K	266	GLY	5.0
1	D	261	GLU	4.9
1	O	254	GLU	4.9
1	R	167	GLU	4.8
1	M	262	GLY	4.8
1	H	254	GLU	4.8
1	E	254	GLU	4.8
1	O	179	VAL	4.7
1	P	229	ARG	4.6
1	O	226	GLY	4.6
1	B	292	GLU	4.6
1	M	165	TYR	4.6
1	O	130	ALA	4.5
1	K	258	ARG	4.5
1	K	229	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	P	228	ILE	4.4
1	B	254	GLU	4.4
1	O	229	ARG	4.4
1	O	52	HIS	4.4
1	K	261	GLU	4.4
1	R	58	ILE	4.4
1	R	251	GLN	4.3
1	H	263	LYS	4.3
1	Q	254	GLU	4.3
1	H	180	GLY	4.3
1	E	285	GLU	4.3
1	K	264	GLY	4.3
1	M	304	ALA	4.2
1	K	224	SER	4.2
1	M	198	PRO	4.2
1	B	289	HIS	4.2
1	M	180	GLY	4.1
1	O	285	GLU	4.1
1	P	237	GLY	4.1
1	E	255	GLU	4.1
1	L	130	ALA	4.1
1	R	182	ARG	4.1
1	F	181	ALA	4.1
1	P	260	TYR	4.1
1	E	194	SER	4.0
1	J	106	THR	4.0
1	E	231	ASP	4.0
1	E	17	GLY	4.0
1	E	203	TYR	4.0
1	P	227	THR	4.0
1	J	107	GLN	4.0
1	N	181	ALA	4.0
1	P	298	ARG	4.0
1	R	226	GLY	3.9
1	R	271	ASP	3.9
1	Q	52	HIS	3.9
1	L	261	GLU	3.9
1	P	16	ILE	3.9
1	R	238	ILE	3.9
1	R	104	ARG	3.9
1	R	228	ILE	3.9
1	H	258	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	P	258	ARG	3.9
1	P	289	HIS	3.8
1	R	216	LYS	3.8
1	K	104	ARG	3.8
1	M	27	VAL	3.8
1	P	256	LEU	3.8
1	O	180	GLY	3.8
1	R	286	ARG	3.8
1	O	288	HIS	3.8
1	M	50	ASP	3.8
1	R	245	TYR	3.8
1	P	167	GLU	3.8
1	R	285	GLU	3.8
1	E	182	ARG	3.8
1	G	309	ARG	3.7
1	M	263	LYS	3.7
1	C	19	TYR	3.7
1	H	179	VAL	3.7
1	O	281	ARG	3.7
1	I	261	GLU	3.7
1	M	32	GLU	3.7
1	G	285	GLU	3.7
1	R	214	GLU	3.7
1	R	175	ARG	3.6
1	J	15	THR	3.6
1	R	247	THR	3.6
1	P	241	LEU	3.6
1	H	226	GLY	3.6
1	A	167	GLU	3.6
1	E	176	ILE	3.6
1	G	289	HIS	3.5
1	M	177	PRO	3.5
1	K	22	ALA	3.5
1	O	32	GLU	3.5
1	P	252	SER	3.5
1	P	192	LYS	3.5
1	R	209	ASP	3.5
1	M	289	HIS	3.5
1	P	26	PHE	3.5
1	Q	292	GLU	3.5
1	O	31	HIS	3.5
1	F	191	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	24	ARG	3.4
1	R	278	GLU	3.4
1	E	289	HIS	3.4
1	H	52	HIS	3.4
1	O	289	HIS	3.4
1	F	190	THR	3.4
1	K	225	GLU	3.4
1	E	52	HIS	3.4
1	P	219	SER	3.4
1	M	281	ARG	3.4
1	O	131	ALA	3.4
1	M	191	LYS	3.4
1	M	211	LYS	3.4
1	G	130	ALA	3.4
1	B	226	GLY	3.4
1	B	107	GLN	3.4
1	P	15	THR	3.4
1	G	167	GLU	3.4
1	O	198	PRO	3.4
1	P	177	PRO	3.4
1	C	15	THR	3.3
1	F	146	ASP	3.3
1	K	255	GLU	3.3
1	M	301	ASP	3.3
1	P	238	ILE	3.3
1	Q	229	ARG	3.3
1	R	177	PRO	3.3
1	K	230	TYR	3.3
1	M	31	HIS	3.3
1	M	293	SER	3.2
1	K	262	GLY	3.2
1	M	278	GLU	3.2
1	M	253	ILE	3.2
1	B	177	PRO	3.2
1	B	300	LEU	3.2
1	K	168	LEU	3.2
1	O	217	ILE	3.2
1	P	271	ASP	3.2
1	M	226	GLY	3.2
1	M	130	ALA	3.2
1	K	226	GLY	3.2
1	J	258	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	3.2
1	A	258	ARG	3.2
1	M	297	ASP	3.1
1	O	161	PHE	3.1
1	R	165	TYR	3.1
1	M	127	PRO	3.1
1	H	194	SER	3.1
1	O	293	SER	3.1
1	Q	53	GLU	3.1
1	L	107	GLN	3.1
1	F	254	GLU	3.1
1	J	130	ALA	3.1
1	K	28	GLU	3.1
1	M	294	GLU	3.1
1	O	312	SER	3.1
1	E	251	GLN	3.1
1	H	15	THR	3.1
1	M	161	PHE	3.1
1	M	196	SER	3.1
1	E	227	THR	3.0
1	M	176	ILE	3.0
1	O	53	GLU	3.0
1	O	167	GLU	3.0
1	R	246	SER	3.0
1	R	293	SER	3.0
1	O	127	PRO	3.0
1	C	262	GLY	3.0
1	O	263	LYS	3.0
1	K	180	GLY	3.0
1	G	305	GLU	3.0
1	O	107	GLN	3.0
1	E	242	LEU	3.0
1	B	127	PRO	3.0
1	P	176	ILE	3.0
1	B	173	GLU	3.0
1	E	130	ALA	3.0
1	A	16	ILE	3.0
1	A	261	GLU	3.0
1	R	59	ARG	3.0
1	Q	107	GLN	2.9
1	G	14	ILE	2.9
1	K	211	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	217	ILE	2.9
1	B	32	GLU	2.9
1	M	78	PHE	2.9
1	F	131	ALA	2.9
1	N	22	ALA	2.9
1	O	300	LEU	2.9
1	R	227	THR	2.9
1	D	52	HIS	2.9
1	K	15	THR	2.9
1	I	32	GLU	2.9
1	M	178	LYS	2.9
1	K	256	LEU	2.9
1	B	285	GLU	2.9
1	M	300	LEU	2.9
1	G	177	PRO	2.9
1	E	56	GLN	2.9
1	D	176	ILE	2.9
1	D	292	GLU	2.9
1	J	167	GLU	2.9
1	M	2	LYS	2.9
1	D	53	GLU	2.8
1	Q	176	ILE	2.8
1	B	258	ARG	2.8
1	F	124	THR	2.8
1	K	201	LYS	2.8
1	E	290	TRP	2.8
1	I	181	ALA	2.8
1	P	250	GLY	2.8
1	L	229	ARG	2.8
1	P	182	ARG	2.8
1	D	107	GLN	2.8
1	M	292	GLU	2.8
1	I	167	GLU	2.8
1	F	128	LEU	2.8
1	M	106	THR	2.8
1	Q	15	THR	2.8
1	L	179	VAL	2.8
1	O	201	LYS	2.8
1	H	28	GLU	2.8
1	E	209	ASP	2.8
1	L	262	GLY	2.8
1	M	210	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	270	ALA	2.7
1	H	299	VAL	2.7
1	K	267	VAL	2.7
1	G	178	LYS	2.7
1	A	145	GLU	2.7
1	D	15	THR	2.7
1	M	77	LEU	2.7
1	D	127	PRO	2.7
1	G	211	LYS	2.7
1	B	31	HIS	2.7
1	M	28	GLU	2.7
1	M	190	THR	2.7
1	P	214	GLU	2.7
1	I	22	ALA	2.7
1	K	294	GLU	2.7
1	P	52	HIS	2.7
1	P	180	GLY	2.7
1	R	237	GLY	2.7
1	R	22	ALA	2.7
1	M	251	GLN	2.7
1	N	285	GLU	2.7
1	M	167	GLU	2.6
1	M	254	GLU	2.6
1	H	182	ARG	2.6
1	P	201	LYS	2.6
1	M	274	GLN	2.6
1	F	226	GLY	2.6
1	E	228	ILE	2.6
1	J	16	ILE	2.6
1	Q	262	GLY	2.6
1	N	289	HIS	2.6
1	Q	32	GLU	2.6
1	M	15	THR	2.6
1	P	217	ILE	2.6
1	K	271	ASP	2.6
1	G	180	GLY	2.6
1	H	192	LYS	2.6
1	R	225	GLU	2.6
1	H	31	HIS	2.6
1	O	261	GLU	2.6
1	N	179	VAL	2.6
1	E	195	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	SER	2.6
1	F	16	ILE	2.6
1	M	19	TYR	2.6
1	P	285	GLU	2.6
1	E	281	ARG	2.6
1	R	196	SER	2.6
1	A	15	THR	2.5
1	P	240	ASN	2.5
1	Q	198	PRO	2.5
1	A	32	GLU	2.5
1	B	165	TYR	2.5
1	N	52	HIS	2.5
1	R	313	GLU	2.5
1	F	2	LYS	2.5
1	M	261	GLU	2.5
1	R	240	ASN	2.5
1	P	209	ASP	2.5
1	G	237	GLY	2.5
1	B	28	GLU	2.5
1	G	294	GLU	2.5
1	D	289	HIS	2.5
1	O	178	LYS	2.5
1	O	181	ALA	2.5
1	P	174	ALA	2.5
1	A	94	GLN	2.5
1	O	60	ARG	2.5
1	M	53	GLU	2.5
1	R	28	GLU	2.5
1	F	169	PHE	2.5
1	F	258	ARG	2.5
1	H	229	ARG	2.5
1	B	52	HIS	2.5
1	B	62	ALA	2.5
1	C	131	ALA	2.5
1	L	145	GLU	2.5
1	H	2	LYS	2.5
1	P	203	TYR	2.5
1	F	261	GLU	2.5
1	I	285	GLU	2.5
1	L	127	PRO	2.5
1	R	266	GLY	2.5
1	O	177	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	202	ALA	2.4
1	I	179	VAL	2.4
1	K	268	PHE	2.4
1	F	262	GLY	2.4
1	I	281	ARG	2.4
1	E	294	GLU	2.4
1	Q	255	GLU	2.4
1	B	182	ARG	2.4
1	A	289	HIS	2.4
1	Q	130	ALA	2.4
1	L	178	LYS	2.4
1	P	32	GLU	2.4
1	R	211	LYS	2.4
1	L	144	GLY	2.4
1	F	211	LYS	2.4
1	J	198	PRO	2.4
1	G	181	ALA	2.4
1	M	197	ASP	2.4
1	Q	263	LYS	2.4
1	D	229	ARG	2.4
1	L	281	ARG	2.4
1	P	255	GLU	2.4
1	M	230	TYR	2.3
1	G	52	HIS	2.3
1	E	196	SER	2.3
1	R	192	LYS	2.3
1	M	199	ASN	2.3
1	O	38	CYS	2.3
1	N	94	GLN	2.3
1	E	177	PRO	2.3
1	L	131	ALA	2.3
1	F	281	ARG	2.3
1	H	225	GLU	2.3
1	N	261	GLU	2.3
1	B	53	GLU	2.3
1	M	285	GLU	2.3
1	R	203	TYR	2.3
1	A	182	ARG	2.3
1	C	130	ALA	2.3
1	D	130	ALA	2.3
1	G	210	ALA	2.3
1	M	201	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	104	ARG	2.3
1	H	198	PRO	2.3
1	R	63	ALA	2.3
1	H	167	GLU	2.3
1	H	292	GLU	2.3
1	B	237	GLY	2.3
1	L	176	ILE	2.3
1	F	179	VAL	2.3
1	H	261	GLU	2.3
1	L	128	LEU	2.3
1	R	242	LEU	2.3
1	E	133	ILE	2.3
1	R	217	ILE	2.3
1	O	50	ASP	2.3
1	C	128	LEU	2.3
1	O	128	LEU	2.3
1	P	127	PRO	2.3
1	H	22	ALA	2.3
1	M	65	TYR	2.3
1	E	298	ARG	2.3
1	K	26	PHE	2.3
1	O	200	PRO	2.2
1	H	190	THR	2.2
1	M	38	CYS	2.2
1	P	259	GLN	2.2
1	A	241	LEU	2.2
1	C	127	PRO	2.2
1	L	52	HIS	2.2
1	N	254	GLU	2.2
1	P	293	SER	2.2
1	R	54	LEU	2.2
1	R	15	THR	2.2
1	M	209	ASP	2.2
1	B	140	ILE	2.2
1	F	176	ILE	2.2
1	O	253	ILE	2.2
1	K	257	GLU	2.2
1	L	126	PRO	2.2
1	D	16	ILE	2.2
1	N	28	GLU	2.2
1	N	178	LYS	2.2
1	P	211	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	198	PRO	2.2
1	F	285	GLU	2.2
1	O	277	ILE	2.2
1	E	63	ALA	2.2
1	G	131	ALA	2.2
1	Q	106	THR	2.2
1	R	250	GLY	2.2
1	B	309	ARG	2.2
1	M	229	ARG	2.2
1	M	296	LEU	2.2
1	M	80	GLN	2.2
1	F	182	ARG	2.2
1	E	246	SER	2.2
1	M	299	VAL	2.2
1	R	253	ILE	2.2
1	A	107	GLN	2.2
1	G	32	GLU	2.2
1	O	191	LYS	2.2
1	R	52	HIS	2.2
1	M	71	ASP	2.2
1	D	22	ALA	2.2
1	L	22	ALA	2.2
1	O	34	ASN	2.1
1	P	216	LYS	2.1
1	R	195	LYS	2.1
1	E	167	GLU	2.1
1	R	276	VAL	2.1
1	E	271	ASP	2.1
1	M	237	GLY	2.1
1	K	246	SER	2.1
1	O	225	GLU	2.1
1	G	128	LEU	2.1
1	R	289	HIS	2.1
1	E	258	ARG	2.1
1	H	104	ARG	2.1
1	N	258	ARG	2.1
1	M	131	ALA	2.1
1	O	173	GLU	2.1
1	H	176	ILE	2.1
1	G	182	ARG	2.1
1	I	258	ARG	2.1
1	F	130	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	254	GLU	2.1
1	K	285	GLU	2.1
1	R	94	GLN	2.1
1	E	26	PHE	2.1
1	A	237	GLY	2.1
1	K	209	ASP	2.1
1	O	2	LYS	2.1
1	Q	140	ILE	2.1
1	H	127	PRO	2.1
1	P	130	ALA	2.1
1	H	107	GLN	2.1
1	I	107	GLN	2.1
1	R	274	GLN	2.1
1	H	178	LYS	2.1
1	D	128	LEU	2.1
1	F	127	PRO	2.1
1	J	52	HIS	2.1
1	L	133	ILE	2.1
1	N	154	THR	2.1
1	B	255	GLU	2.1
1	F	53	GLU	2.1
1	G	28	GLU	2.1
1	I	94	GLN	2.1
1	M	146	ASP	2.1
1	N	26	PHE	2.1
1	N	180	GLY	2.1
1	K	248	LEU	2.1
1	I	253	ILE	2.1
1	P	183	ILE	2.1
1	C	229	ARG	2.1
1	N	182	ARG	2.1
1	P	104	ARG	2.1
1	A	106	THR	2.1
1	C	254	GLU	2.1
1	P	146	ASP	2.1
1	M	9	GLN	2.0
1	P	242	LEU	2.0
1	G	258	ARG	2.0
1	F	294	GLU	2.0
1	H	145	GLU	2.0
1	I	130	ALA	2.0
1	P	295	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	226	GLY	2.0
1	E	277	ILE	2.0
1	I	198	PRO	2.0
1	K	47	VAL	2.0
1	L	177	PRO	2.0
1	G	175	ARG	2.0
1	R	183	ILE	2.0
1	G	261	GLU	2.0
1	H	98	TYR	2.0
1	K	265	TYR	2.0
1	O	145	GLU	2.0
1	M	303	GLY	2.0
1	N	15	THR	2.0
1	P	249	SER	2.0
1	D	179	VAL	2.0
1	L	167	GLU	2.0
1	M	159	GLU	2.0
1	H	131	ALA	2.0
1	H	201	LYS	2.0
1	N	148	LYS	2.0
1	E	268	PHE	2.0
1	B	104	ARG	2.0
1	H	23	LEU	2.0
1	M	206	LEU	2.0
1	R	298	ARG	2.0
1	D	118	VAL	2.0
1	N	177	PRO	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
4	AMP	P	1003	23/23	0.50	0.84	5.80	54,60,69,70	23
4	AMP	R	1003	23/23	0.27	0.78	4.99	49,56,66,68	23
4	AMP	D	1003	23/23	0.63	0.63	4.97	33,42,54,56	23
4	AMP	K	1003	23/23	0.54	0.57	4.81	47,55,60,61	23
4	AMP	M	1003	23/23	0.76	0.60	4.37	20,20,20,20	0
4	AMP	J	1003	23/23	0.77	0.51	3.72	29,37,48,49	23
4	AMP	F	1003	23/23	0.50	0.56	3.65	39,47,56,58	23
2	TRP	B	1001	15/15	0.91	0.37	3.61	29,44,76,106	15
4	AMP	Q	1003	23/23	0.75	0.40	3.31	22,37,51,53	23
4	AMP	O	1003	23/23	0.75	0.41	3.12	34,41,47,48	23
4	AMP	G	1003	23/23	0.84	0.43	3.08	41,47,51,53	23
4	AMP	C	1003	23/23	0.69	0.43	3.07	21,30,43,44	23
2	TRP	O	1001	15/15	0.87	0.33	3.01	24,42,70,106	15
4	AMP	L	1003	23/23	0.77	0.43	2.94	24,37,46,47	23
4	AMP	B	1003	23/23	0.75	0.40	2.73	34,43,47,49	23
4	AMP	H	1003	23/23	0.65	0.48	2.49	45,50,52,53	23
4	AMP	A	1003	23/23	0.82	0.39	2.43	38,41,48,50	23
4	AMP	I	1003	23/23	0.76	0.40	2.23	22,28,41,42	23
2	TRP	H	1001	15/15	0.94	0.29	2.13	20,36,73,103	15
4	AMP	N	1003	23/23	0.72	0.45	2.10	19,29,47,48	23
4	AMP	E	1003	23/23	0.62	0.56	2.06	42,50,56,57	23
2	TRP	J	1001	15/15	0.96	0.26	1.95	16,30,62,95	15
2	TRP	M	1001	15/15	0.85	0.34	1.90	21,34,65,103	15
2	TRP	D	1001	15/15	0.94	0.25	1.58	11,32,64,100	15
2	TRP	R	1001	15/15	0.93	0.29	1.33	12,44,70,106	15
2	TRP	N	1001	15/15	0.97	0.23	1.23	14,29,61,100	15
2	TRP	P	1001	15/15	0.94	0.29	1.18	18,32,70,99	15
2	TRP	A	1001	15/15	0.95	0.23	0.69	22,34,61,104	15
2	TRP	I	1001	15/15	0.96	0.22	0.64	16,37,63,103	15
2	TRP	Q	1001	15/15	0.93	0.21	0.54	20,34,69,98	15
2	TRP	E	1001	15/15	0.94	0.24	0.49	5,25,52,93	15
2	TRP	F	1001	15/15	0.96	0.23	0.44	12,37,65,99	15
2	TRP	C	1001	15/15	0.96	0.23	0.26	20,37,69,101	15
2	TRP	G	1001	15/15	0.95	0.23	0.10	23,46,73,106	15
3	PO4	O	1002	5/5	0.87	0.24	-0.08	41,44,46,47	5
2	TRP	L	1001	15/15	0.95	0.21	-0.11	20,35,69,101	15
3	PO4	I	1002	5/5	0.93	0.20	-0.40	47,50,53,53	5
3	PO4	K	1002	5/5	0.92	0.21	-0.54	64,67,70,71	5
2	TRP	K	1001	15/15	0.96	0.18	-0.57	16,32,62,101	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	1002	5/5	0.97	0.17	-0.73	39,43,45,45	5
3	PO4	G	1002	5/5	0.96	0.14	-1.52	50,53,56,56	5
3	PO4	C	1002	5/5	0.95	0.16	-1.63	42,45,48,49	5
3	PO4	J	1002	5/5	0.96	0.12	-1.73	65,68,71,72	0
3	PO4	D	1002	5/5	0.96	0.12	-1.94	51,54,56,59	0
3	PO4	N	1002	5/5	0.95	0.12	-2.00	52,55,57,59	0
3	PO4	Q	1002	5/5	0.97	0.11	-2.15	34,37,40,42	5
3	PO4	H	1002	5/5	0.94	0.11	-2.28	46,49,52,54	5
3	PO4	B	1002	5/5	0.97	0.10	-3.39	48,51,54,54	5
3	PO4	L	1002	5/5	0.98	0.08	-3.82	57,60,62,63	0
3	PO4	M	1002	5/5	0.95	0.36	-	20,20,20,20	0
3	PO4	E	1002	5/5	0.86	0.23	-	75,78,80,81	5
3	PO4	R	1002	5/5	0.83	0.21	-	76,79,82,83	5
3	PO4	F	1002	5/5	0.94	0.15	-	51,54,58,60	0
3	PO4	P	1002	5/5	0.72	0.34	-	104,107,110,111	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.