



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:04 AM GMT

PDB ID : 3KLE  
Title : Crystal structure of AZT-resistant HIV-1 Reverse Transcriptase crosslinked to a DSDNA with a bound excision product, AZTPPPPA  
Authors : Tu, X.; Das, K.; Sarafianos, S.G.; Arnold, E.  
Deposited on : 2009-11-07  
Resolution : 3.20 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

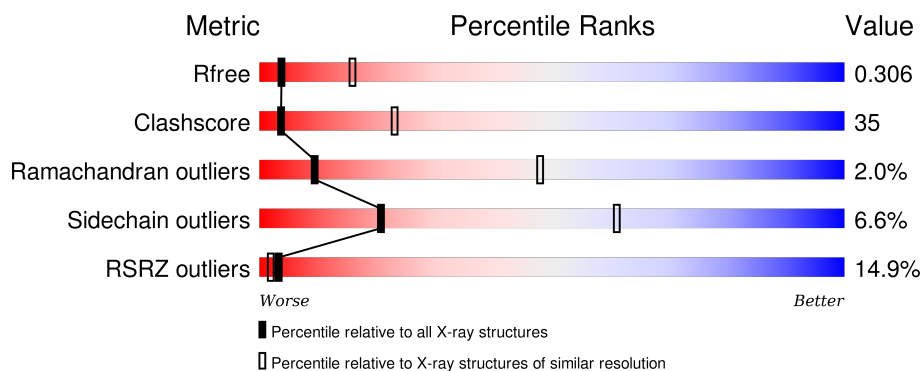
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	562	<div> <div>41%</div> <div>53%</div> <div>6%</div> </div>
1	E	562	<div> <div>40%</div> <div>53%</div> <div>6%</div> </div>
1	I	562	<div> <div>16%</div> <div>39%</div> <div>55%</div> <div>6%</div> </div>
1	M	562	<div> <div>35%</div> <div>41%</div> <div>53%</div> <div>6%</div> </div>
2	B	437	<div> <div>3%</div> <div>46%</div> <div>46%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	437	
2	J	437	
2	N	437	
3	C	27	
3	G	27	
3	K	27	
3	O	27	
4	D	21	
4	H	21	
4	L	21	
4	P	21	

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
7	GOL	B	438	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 36120 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	E	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	I	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	M	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	41	LEU	MET	ENGINEERED	UNP P03366
A	67	ASN	ASP	ENGINEERED	UNP P03366
A	70	ARG	LYS	ENGINEERED	UNP P03366
A	215	TYR	THR	ENGINEERED	UNP P03366
A	219	GLN	LYS	ENGINEERED	UNP P03366
A	258	CYS	GLN	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366
A	559	VAL	ILE	SEE REMERK 999	UNP P03366
E	-1	MET	-	EXPRESSION TAG	UNP P03366
E	0	VAL	-	EXPRESSION TAG	UNP P03366
E	41	LEU	MET	ENGINEERED	UNP P03366
E	67	ASN	ASP	ENGINEERED	UNP P03366
E	70	ARG	LYS	ENGINEERED	UNP P03366
E	215	TYR	THR	ENGINEERED	UNP P03366
E	219	GLN	LYS	ENGINEERED	UNP P03366
E	258	CYS	GLN	ENGINEERED	UNP P03366
E	280	SER	CYS	ENGINEERED	UNP P03366
E	559	VAL	ILE	SEE REMERK 999	UNP P03366
I	-1	MET	-	EXPRESSION TAG	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	VAL	-	EXPRESSION TAG	UNP P03366
I	41	LEU	MET	ENGINEERED	UNP P03366
I	67	ASN	ASP	ENGINEERED	UNP P03366
I	70	ARG	LYS	ENGINEERED	UNP P03366
I	215	TYR	THR	ENGINEERED	UNP P03366
I	219	GLN	LYS	ENGINEERED	UNP P03366
I	258	CYS	GLN	ENGINEERED	UNP P03366
I	280	SER	CYS	ENGINEERED	UNP P03366
I	559	VAL	ILE	SEE REMERK 999	UNP P03366
M	-1	MET	-	EXPRESSION TAG	UNP P03366
M	0	VAL	-	EXPRESSION TAG	UNP P03366
M	41	LEU	MET	ENGINEERED	UNP P03366
M	67	ASN	ASP	ENGINEERED	UNP P03366
M	70	ARG	LYS	ENGINEERED	UNP P03366
M	215	TYR	THR	ENGINEERED	UNP P03366
M	219	GLN	LYS	ENGINEERED	UNP P03366
M	258	CYS	GLN	ENGINEERED	UNP P03366
M	280	SER	CYS	ENGINEERED	UNP P03366
M	559	VAL	ILE	SEE REMERK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	0	0
			3462	2248	576	632	6			
2	F	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			
2	J	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			
2	N	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366
B	429	GLY	-	EXPRESSION TAG	UNP P03366
B	430	GLY	-	EXPRESSION TAG	UNP P03366
B	431	HIS	-	EXPRESSION TAG	UNP P03366
B	432	HIS	-	EXPRESSION TAG	UNP P03366
B	433	HIS	-	EXPRESSION TAG	UNP P03366
B	434	HIS	-	EXPRESSION TAG	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	435	HIS	-	EXPRESSION TAG	UNP P03366
B	436	HIS	-	EXPRESSION TAG	UNP P03366
B	437	HIS	-	EXPRESSION TAG	UNP P03366
F	280	SER	CYS	ENGINEERED	UNP P03366
F	429	GLY	-	EXPRESSION TAG	UNP P03366
F	430	GLY	-	EXPRESSION TAG	UNP P03366
F	431	HIS	-	EXPRESSION TAG	UNP P03366
F	432	HIS	-	EXPRESSION TAG	UNP P03366
F	433	HIS	-	EXPRESSION TAG	UNP P03366
F	434	HIS	-	EXPRESSION TAG	UNP P03366
F	435	HIS	-	EXPRESSION TAG	UNP P03366
F	436	HIS	-	EXPRESSION TAG	UNP P03366
F	437	HIS	-	EXPRESSION TAG	UNP P03366
J	280	SER	CYS	ENGINEERED	UNP P03366
J	429	GLY	-	EXPRESSION TAG	UNP P03366
J	430	GLY	-	EXPRESSION TAG	UNP P03366
J	431	HIS	-	EXPRESSION TAG	UNP P03366
J	432	HIS	-	EXPRESSION TAG	UNP P03366
J	433	HIS	-	EXPRESSION TAG	UNP P03366
J	434	HIS	-	EXPRESSION TAG	UNP P03366
J	435	HIS	-	EXPRESSION TAG	UNP P03366
J	436	HIS	-	EXPRESSION TAG	UNP P03366
J	437	HIS	-	EXPRESSION TAG	UNP P03366
N	280	SER	CYS	ENGINEERED	UNP P03366
N	429	GLY	-	EXPRESSION TAG	UNP P03366
N	430	GLY	-	EXPRESSION TAG	UNP P03366
N	431	HIS	-	EXPRESSION TAG	UNP P03366
N	432	HIS	-	EXPRESSION TAG	UNP P03366
N	433	HIS	-	EXPRESSION TAG	UNP P03366
N	434	HIS	-	EXPRESSION TAG	UNP P03366
N	435	HIS	-	EXPRESSION TAG	UNP P03366
N	436	HIS	-	EXPRESSION TAG	UNP P03366
N	437	HIS	-	EXPRESSION TAG	UNP P03366

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			
3	G	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			
3	K	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			

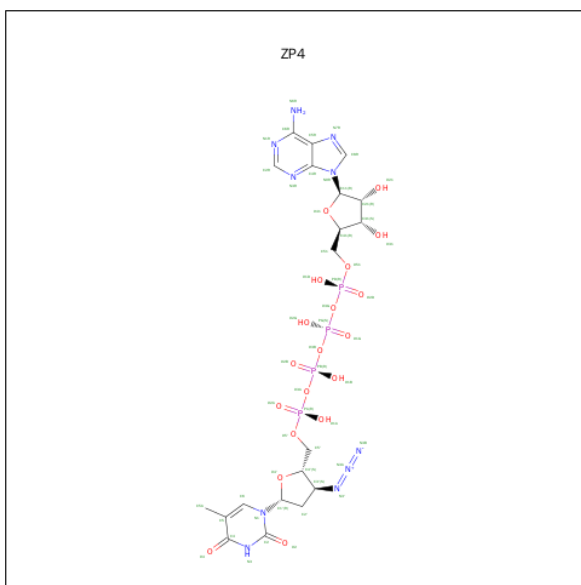
- Molecule 4 is a DNA chain called DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(2DA))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	H	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	L	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	P	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

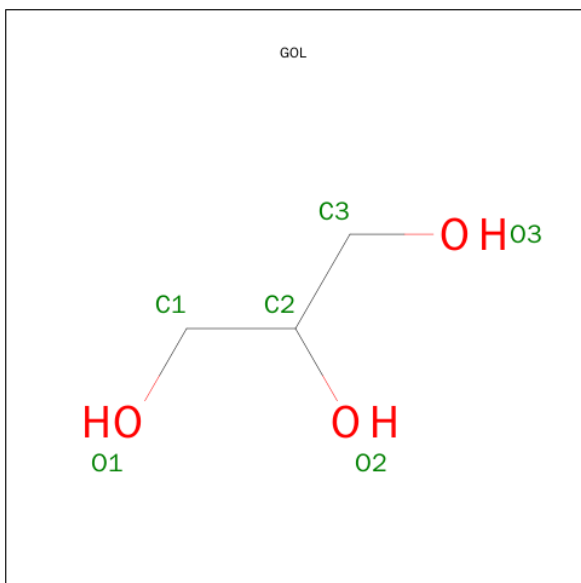
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		
5	M	2	Total	Mg	0	0
			2	2		
5	E	2	Total	Mg	0	0
			2	2		

- Molecule 6 is [((((2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL)METHOXY-HYDROXY-PHOSPHORYL)OXY-HYDROXY-PHOSPHORYL)OXY-HYDROXY-PHOSPHORYL] [(2S,3S,5R)-3-AZIDO-5-(5-METHYL-2,4-DIOXO-PYRIMIDIN-1-YL)OXOLAN-2-YL]METHYL HYDROGEN PHOSPHATE (three-letter code: ZP4) (formula: C<sub>20</sub>H<sub>28</sub>N<sub>10</sub>O<sub>19</sub>P<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
6	E	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
6	I	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
6	M	1	Total	C	N	O	P	0	0
			53	20	10	19	4		

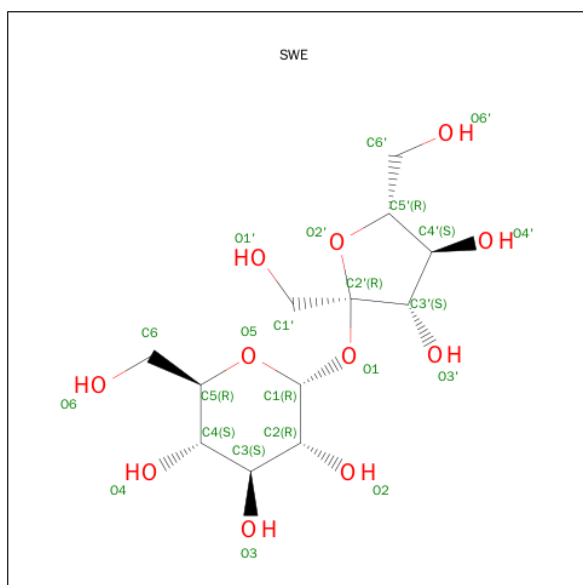
- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ALPHA-D-FRUCTOFURANOSYL ALPHA-D-GLUCOPYRANOSIDE (three-letter code: SWE) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	J	1	Total	C	O	0	0
			23	12	11		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	18	Total	O	0	0
			18	18		
9	B	10	Total	O	0	0
			10	10		
9	E	12	Total	O	0	0
			12	12		
9	F	10	Total	O	0	0
			10	10		
9	I	5	Total	O	0	0
			5	5		
9	J	14	Total	O	0	0
			14	14		

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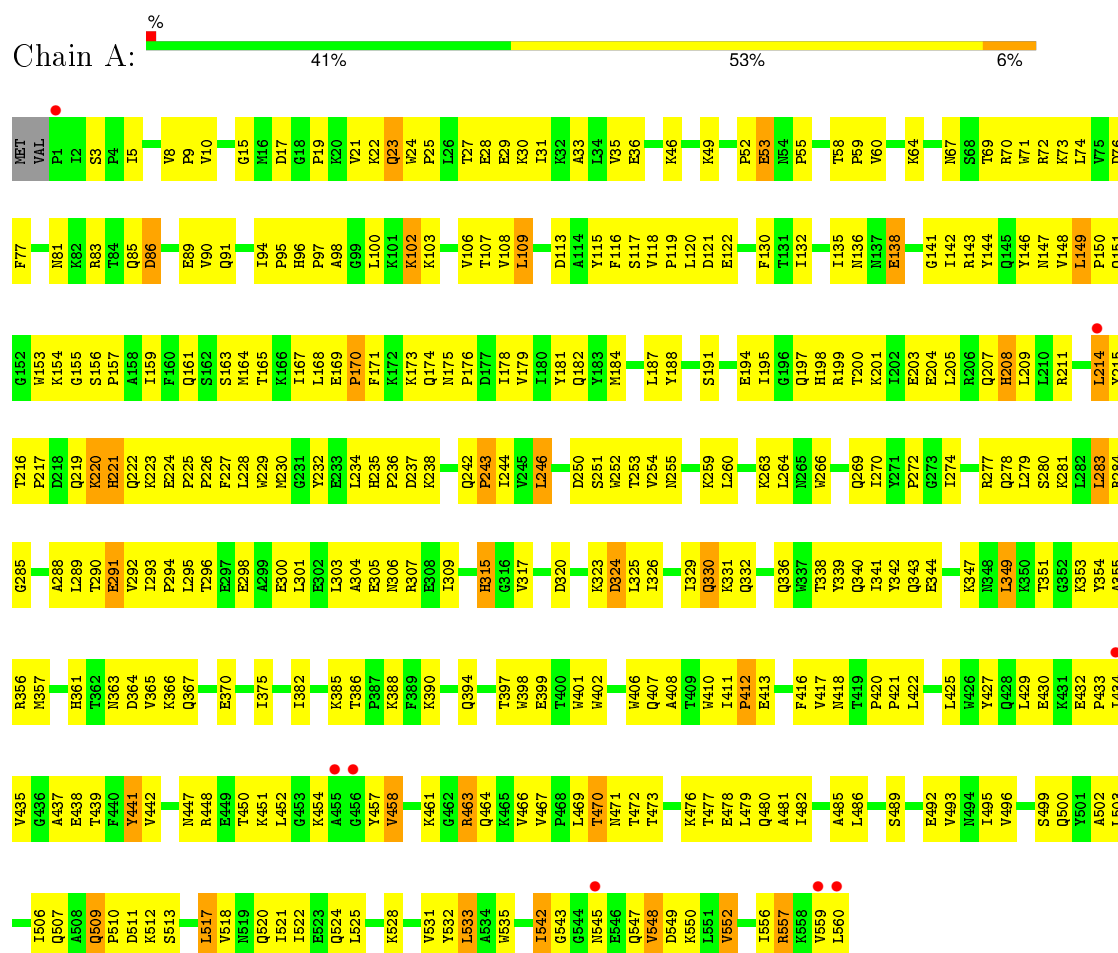
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	3	Total 3	O 3	0	0
9	N	8	Total 8	O 8	0	0
9	C	2	Total 2	O 2	0	0
9	D	2	Total 2	O 2	0	0
9	G	1	Total 1	O 1	0	0
9	H	1	Total 1	O 1	0	0
9	K	1	Total 1	O 1	0	0
9	L	1	Total 1	O 1	0	0
9	O	4	Total 4	O 4	0	0
9	P	1	Total 1	O 1	0	0

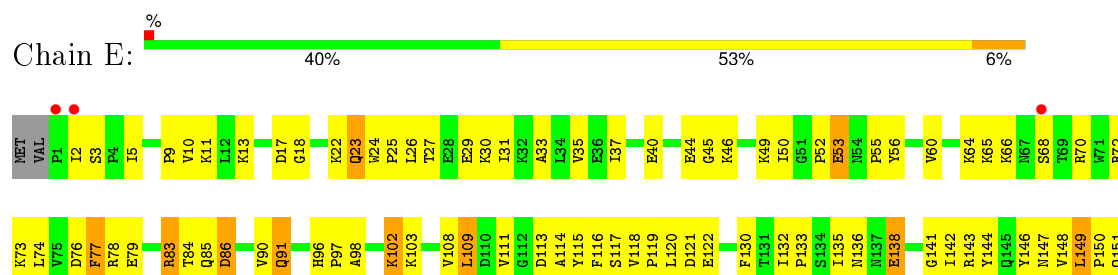
### 3 Residue-property plots

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

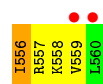
#### • Molecule 1: Reverse transcriptase/ribonuclease H



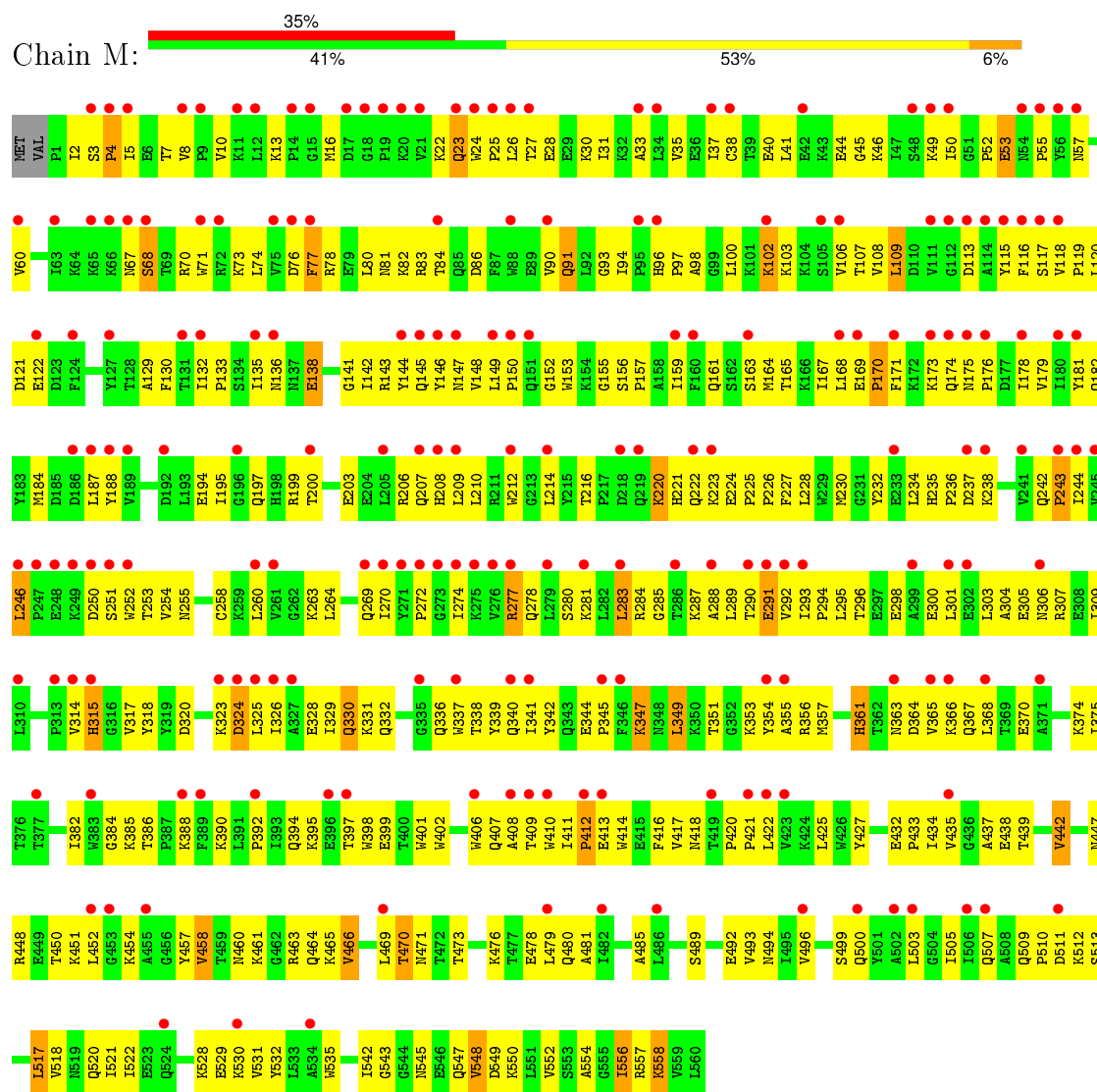
#### • Molecule 1: Reverse transcriptase/ribonuclease H



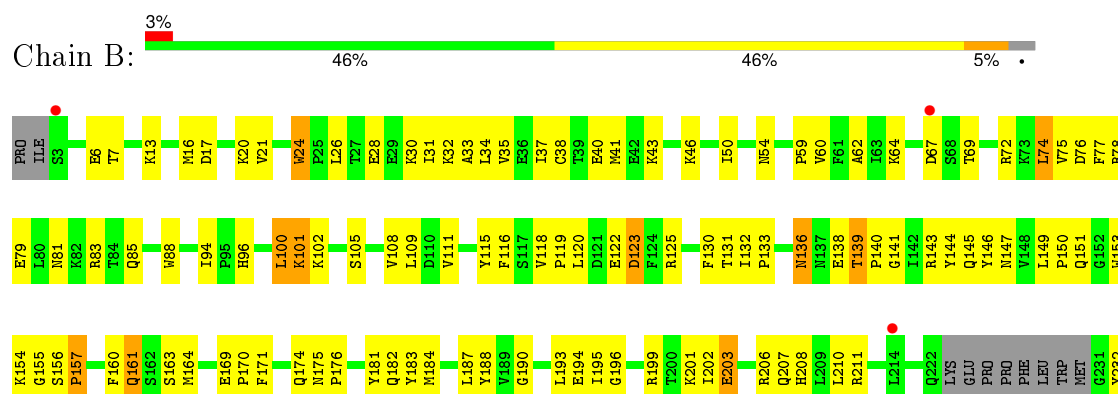


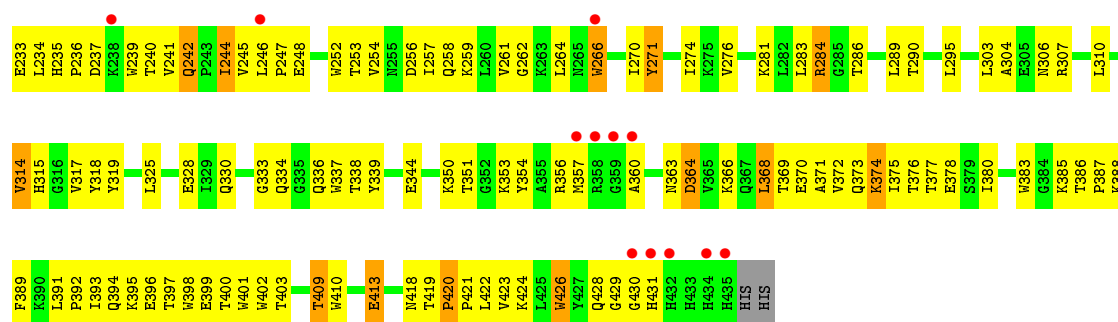


• Molecule 1: Reverse transcriptase/ribonuclease H

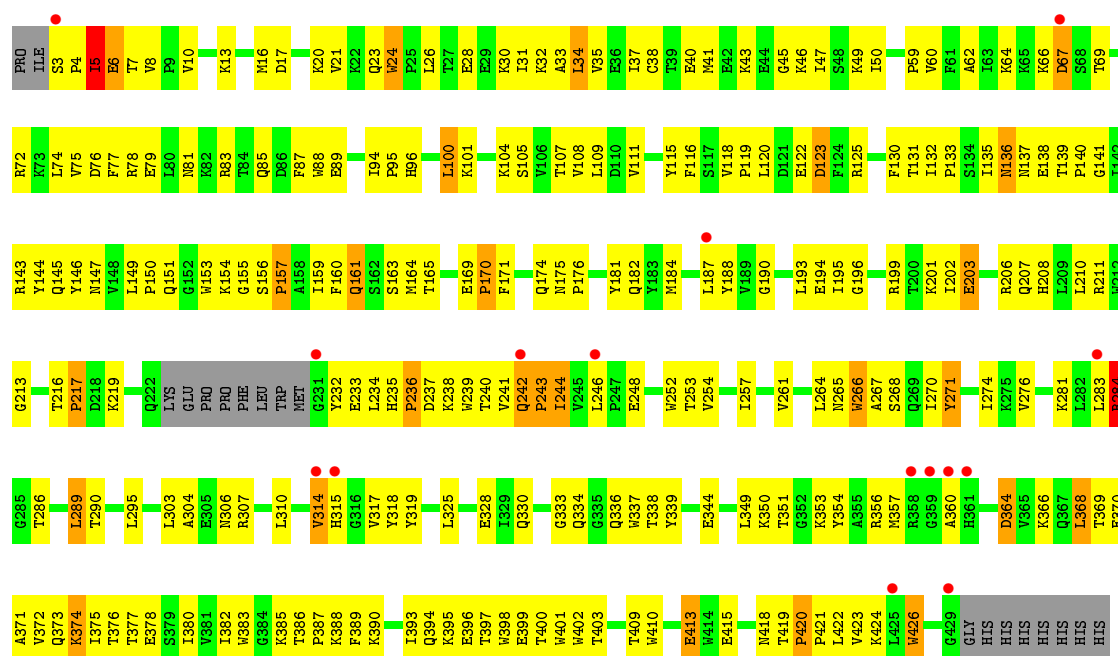


• Molecule 2: p51 RT

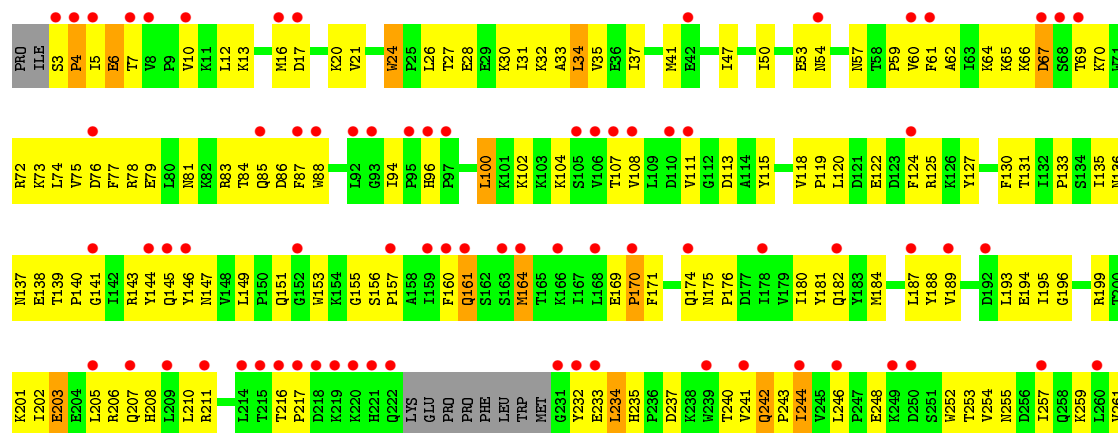
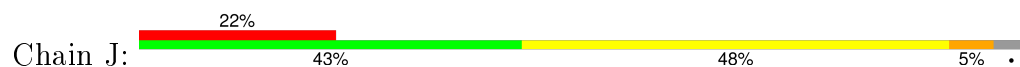


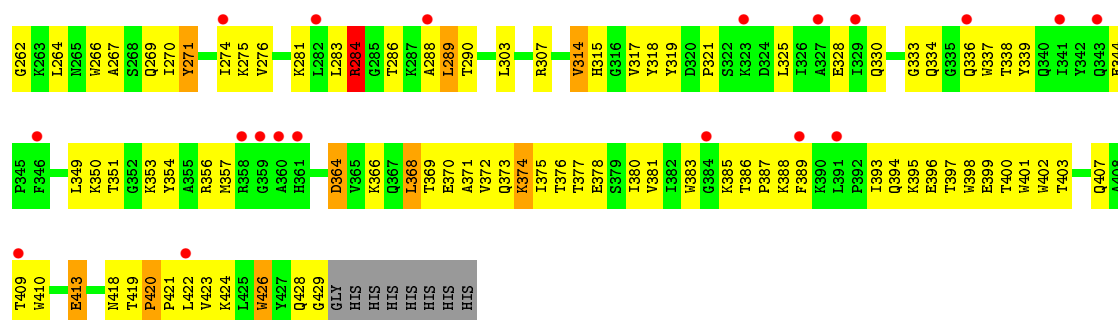


• Molecule 2: p51 RT

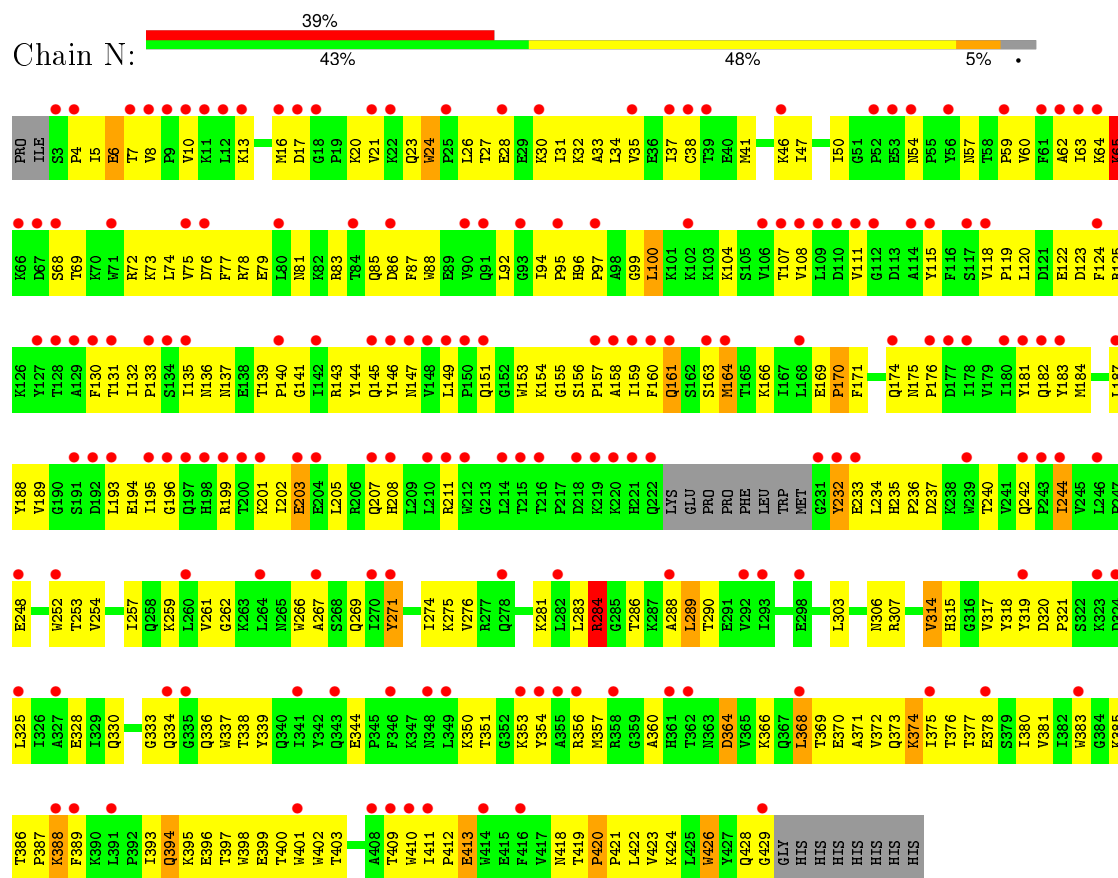


• Molecule 2: p51 RT





- Molecule 2: p51 RT



- Molecule 3: DNA (25-MER)



- Molecule 3: DNA (25-MER)



- Molecule 3: DNA (25-MER)

Chain K: 



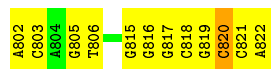
- Molecule 3: DNA (25-MER)

Chain O: 



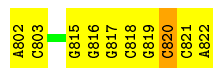
- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(2DA))-3')

Chain D: 



- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(2DA))-3')

Chain H: 



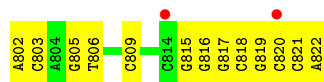
- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(2DA))-3')

Chain L: 



- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(2DA))-3')

Chain P: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.74Å 283.33Å 155.23Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	24.83 – 3.20 24.83 – 3.18	Depositor EDS
% Data completeness (in resolution range)	90.4 (24.83-3.20) 88.8 (24.83-3.18)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.17Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.280 , 0.308 0.280 , 0.306	Depositor DCC
$R_{free}$ test set	1992 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 12.8	EDS
Estimated twinning fraction	0.279 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 100886 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	36120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SWE, ZP4, 2DA, MRG

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	0.56	0/4679	0.70	2/6357 (0.0%)
1	E	0.59	0/4679	0.71	2/6357 (0.0%)
1	I	0.42	0/4679	0.61	0/6357
1	M	0.42	0/4679	0.61	2/6357 (0.0%)
2	B	0.63	0/3559	0.71	0/4838
2	F	0.62	0/3531	0.71	0/4800
2	J	0.44	0/3531	0.64	0/4800
2	N	0.42	0/3531	0.62	0/4800
3	C	0.88	0/579	0.93	0/893
3	G	0.96	0/579	0.93	0/893
3	K	0.56	0/579	0.81	0/893
3	O	0.56	0/579	0.81	0/893
4	D	0.92	0/424	0.90	0/649
4	H	0.87	0/424	0.93	0/649
4	L	0.56	0/424	0.88	0/649
4	P	0.53	0/424	0.85	0/649
All	All	0.55	0/36880	0.69	6/50834 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	G	0	1
3	K	0	1
3	O	0	1
4	D	0	1
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	442	VAL	CB-CA-C	-5.99	100.03	111.40
1	A	542	ILE	CB-CA-C	-5.82	99.95	111.60
1	M	68	SER	CB-CA-C	-5.54	99.57	110.10
1	A	463	ARG	CB-CA-C	-5.51	99.39	110.40
1	E	492	GLU	N-CA-C	-5.31	96.66	111.00
1	E	205	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	705	DA	Sidechain
4	D	820	DC	Sidechain
3	G	705	DA	Sidechain
4	H	820	DC	Sidechain
3	K	705	DA	Sidechain
3	O	705	DA	Sidechain

## 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	4560	0	4627	358	0
1	E	4560	0	4627	359	0
1	I	4560	0	4627	385	0
1	M	4560	0	4628	344	0
2	B	3462	0	3462	236	0
2	F	3434	0	3450	260	0
2	J	3434	0	3450	273	0
2	N	3434	0	3450	253	0
3	C	515	0	280	24	0
3	G	515	0	280	25	0
3	K	515	0	280	27	0
3	O	515	0	280	24	0
4	D	427	0	242	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	427	0	242	11	0
4	L	427	0	242	12	0
4	P	427	0	243	16	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
5	I	2	0	0	0	0
5	M	2	0	0	0	0
6	A	53	0	24	10	0
6	E	53	0	24	9	0
6	I	53	0	24	4	0
6	M	53	0	24	7	0
7	B	6	0	8	0	0
7	F	6	0	8	0	0
8	J	23	0	22	5	0
9	A	18	0	0	0	0
9	B	10	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	12	0	0	0	0
9	F	10	0	0	1	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	5	0	0	1	0
9	J	14	0	0	5	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	M	3	0	0	0	0
9	N	8	0	0	3	0
9	O	4	0	0	0	0
9	P	1	0	0	1	0
All	All	36120	0	34544	2498	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 35.

All (2498) 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:I:441:TYR:CD1	1:I:544:GLY:HA3	1.70	1.25
1:I:286:THR:O	1:I:287:LYS:HG2	1.44	1.16
2:F:125:ARG:HD3	2:F:147:ASN:HA	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:489:SER:HB2	1:I:493:VAL:HG11	1.29	1.14
2:B:79:GLU:HG3	2:B:83:ARG:HH12	0.98	1.14
1:E:489:SER:HB2	1:E:493:VAL:HG11	1.27	1.14
2:J:125:ARG:HD3	2:J:147:ASN:HA	1.27	1.13
1:E:511:ASP:OD1	1:E:512:LYS:HG3	1.47	1.13
1:I:225:PRO:HB2	1:I:226:PRO:HD3	1.16	1.13
1:M:489:SER:HB2	1:M:493:VAL:HG11	1.28	1.13
1:A:489:SER:HB2	1:A:493:VAL:HG11	1.27	1.12
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.31	1.12
2:F:79:GLU:HG3	2:F:83:ARG:HH12	1.02	1.12
1:E:441:TYR:CD1	1:E:544:GLY:HA3	1.85	1.11
2:B:64:LYS:HE3	2:B:69:THR:HA	1.27	1.11
1:A:157:PRO:O	1:A:161:GLN:HG3	1.49	1.11
2:N:65:LYS:HB2	2:N:68:SER:HB2	1.34	1.10
2:N:125:ARG:HD3	2:N:147:ASN:HA	1.32	1.09
2:N:79:GLU:HG3	2:N:83:ARG:HH12	1.02	1.09
2:F:64:LYS:HE3	2:F:69:THR:HA	1.34	1.08
1:M:511:ASP:OD1	1:M:512:LYS:HG3	1.53	1.07
2:J:79:GLU:HG3	2:J:83:ARG:HH12	0.99	1.06
2:J:184:MET:SD	2:J:410:TRP:HB3	1.96	1.05
1:I:511:ASP:OD1	1:I:512:LYS:CG	2.05	1.04
1:I:511:ASP:OD1	1:I:512:LYS:HG3	1.58	1.03
1:M:90:VAL:HG22	2:N:140:PRO:HB2	1.39	1.03
2:B:79:GLU:HG3	2:B:83:ARG:NH1	1.74	1.02
2:J:79:GLU:HG3	2:J:83:ARG:NH1	1.75	1.02
1:E:102:LYS:HD2	1:E:102:LYS:H	1.24	1.02
1:I:274:ILE:HG23	1:I:306:ASN:HD21	1.26	1.01
2:F:79:GLU:HG3	2:F:83:ARG:NH1	1.76	1.01
1:I:441:TYR:HD1	1:I:544:GLY:HA3	1.22	1.00
1:E:52:PRO:HA	1:E:143:ARG:HH22	1.25	1.00
2:N:79:GLU:HG3	2:N:83:ARG:NH1	1.77	1.00
1:A:23:GLN:NE2	1:A:60:VAL:H	1.59	0.99
1:A:102:LYS:HD2	1:A:102:LYS:H	1.27	0.99
2:J:5:ILE:HG13	2:J:6:GLU:H	1.24	0.99
1:I:439:THR:HG21	2:J:289:LEU:HD13	1.43	0.99
1:M:274:ILE:HG23	1:M:306:ASN:HD21	1.26	0.98
1:E:293:ILE:HD12	1:E:294:PRO:HD2	1.46	0.97
1:I:103:LYS:HE3	1:I:179:VAL:HG21	1.47	0.96
1:E:277:ARG:NH1	1:E:336:GLN:HG3	1.80	0.96
1:M:23:GLN:NE2	1:M:60:VAL:H	1.64	0.96
1:M:439:THR:HG21	2:N:289:LEU:HD13	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:LYS:HD2	1:M:102:LYS:H	1.32	0.94
1:I:67:ASN:O	1:I:68:SER:HB2	1.68	0.93
2:J:5:ILE:HG13	2:J:6:GLU:N	1.81	0.93
1:A:52:PRO:HA	1:A:143:ARG:HH22	1.29	0.93
2:J:79:GLU:CG	2:J:83:ARG:HH12	1.82	0.93
2:B:79:GLU:CG	2:B:83:ARG:HH12	1.82	0.92
2:J:24:TRP:CZ3	2:J:403:THR:HG21	2.05	0.92
1:I:435:VAL:HA	2:J:290:THR:HG21	1.51	0.91
1:M:225:PRO:HB2	1:M:226:PRO:HD3	1.51	0.91
2:B:30:LYS:HE2	2:B:62:ALA:O	1.71	0.91
1:M:157:PRO:O	1:M:161:GLN:HG3	1.69	0.91
1:I:293:ILE:HD12	1:I:294:PRO:HD2	1.51	0.91
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.52	0.91
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.53	0.90
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.50	0.90
2:F:79:GLU:CG	2:F:83:ARG:HH12	1.85	0.90
2:J:157:PRO:HG2	2:J:184:MET:HA	1.51	0.90
1:I:225:PRO:CB	1:I:226:PRO:HD3	2.00	0.90
1:E:23:GLN:NE2	1:E:60:VAL:H	1.69	0.90
1:I:23:GLN:NE2	1:I:60:VAL:H	1.69	0.90
1:I:225:PRO:HB2	1:I:226:PRO:CD	2.01	0.90
2:N:79:GLU:CG	2:N:83:ARG:HH12	1.85	0.90
2:N:60:VAL:HG12	2:N:75:VAL:HG22	1.54	0.90
1:I:238:LYS:HG2	1:I:315:HIS:ND1	1.87	0.89
1:E:157:PRO:O	1:E:161:GLN:HG3	1.73	0.89
1:M:67:ASN:O	1:M:68:SER:HB2	1.70	0.89
1:M:435:VAL:HA	2:N:290:THR:HG21	1.54	0.89
1:I:155:GLY:O	1:I:159:ILE:HG12	1.73	0.88
1:M:135:ILE:HD12	1:M:135:ILE:H	1.36	0.88
2:F:60:VAL:HG12	2:F:75:VAL:HG22	1.53	0.88
1:E:432:GLU:HG3	1:E:433:PRO:HD2	1.55	0.88
1:I:558:LYS:HG2	1:I:559:VAL:H	1.35	0.88
2:F:244:ILE:HD13	2:F:244:ILE:H	1.38	0.88
2:J:60:VAL:HG12	2:J:75:VAL:HG22	1.55	0.88
1:I:277:ARG:NH1	1:I:336:GLN:HG3	1.89	0.88
2:N:64:LYS:HE3	2:N:69:THR:HA	1.56	0.88
1:E:439:THR:HG21	2:F:289:LEU:HD13	1.56	0.87
2:N:111:VAL:HG11	2:N:187:LEU:HD22	1.53	0.87
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.53	0.87
1:A:260:LEU:HD21	1:A:303:LEU:HD23	1.54	0.87
1:M:103:LYS:HE3	1:M:179:VAL:HG21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:261:VAL:HG13	2:F:276:VAL:HG21	1.53	0.87
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.56	0.87
1:I:157:PRO:O	1:I:161:GLN:HG3	1.74	0.87
1:A:485:ALA:O	1:A:489:SER:HB3	1.74	0.87
2:N:157:PRO:HG2	2:N:184:MET:HA	1.54	0.87
1:E:49:LYS:HE3	1:E:142:ILE:HD12	1.57	0.87
1:M:432:GLU:HG3	1:M:433:PRO:HD2	1.56	0.86
1:A:221:HIS:HE1	1:A:228:LEU:HB2	1.40	0.85
2:F:30:LYS:HE2	2:F:62:ALA:O	1.76	0.85
2:B:244:ILE:HD13	2:B:244:ILE:H	1.41	0.85
2:N:96:HIS:HE1	2:N:381:VAL:O	1.59	0.85
1:E:207:GLN:NE2	1:E:210:LEU:HD23	1.91	0.85
1:A:135:ILE:H	1:A:135:ILE:HD12	1.39	0.85
2:F:111:VAL:HG11	2:F:187:LEU:HD22	1.58	0.85
1:I:224:GLU:O	1:I:227:PHE:CE2	2.30	0.85
1:I:382:ILE:O	2:J:136:ASN:HB2	1.76	0.84
1:A:277:ARG:NH1	1:A:336:GLN:HG3	1.92	0.84
2:F:100:LEU:H	2:F:100:LEU:HD23	1.40	0.84
1:M:293:ILE:HD12	1:M:294:PRO:HD2	1.59	0.84
2:N:171:PHE:HB2	2:N:208:HIS:ND1	1.91	0.84
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.12	0.84
1:I:286:THR:C	1:I:287:LYS:HG2	1.97	0.84
1:E:529:GLU:O	1:E:530:LYS:HG3	1.78	0.84
1:I:163:SER:O	1:I:167:ILE:HD13	1.77	0.84
2:B:428:GLN:HG2	2:B:429:GLY:H	1.41	0.84
2:J:234:LEU:H	2:J:234:LEU:HD12	1.43	0.84
1:I:224:GLU:O	1:I:227:PHE:CZ	2.30	0.84
2:F:157:PRO:HG2	2:F:184:MET:HA	1.58	0.84
1:E:485:ALA:O	1:E:489:SER:HB3	1.78	0.83
2:B:13:LYS:O	2:B:16:MET:HB2	1.78	0.83
2:J:244:ILE:HD13	2:J:244:ILE:H	1.40	0.83
1:E:220:LYS:O	1:E:220:LYS:HD2	1.77	0.83
2:J:261:VAL:HG13	2:J:276:VAL:HG21	1.61	0.83
2:B:157:PRO:HG2	2:B:184:MET:HA	1.60	0.83
1:M:503:LEU:O	1:M:507:GLN:HG3	1.79	0.82
1:I:135:ILE:HD12	1:I:135:ILE:H	1.43	0.82
1:I:432:GLU:HG3	1:I:433:PRO:HD2	1.59	0.82
1:M:221:HIS:CE1	1:M:228:LEU:H	1.97	0.82
2:J:171:PHE:HB2	2:J:208:HIS:ND1	1.93	0.82
2:J:13:LYS:O	2:J:16:MET:HB2	1.78	0.82
1:E:135:ILE:HD12	1:E:135:ILE:H	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LEU:H	2:B:100:LEU:HD23	1.43	0.82
2:B:171:PHE:HB2	2:B:208:HIS:ND1	1.95	0.82
1:E:458:VAL:HG12	1:E:548:VAL:HG22	1.61	0.82
1:A:244:ILE:HD11	1:A:263:LYS:HG3	1.62	0.82
1:I:558:LYS:HG2	1:I:559:VAL:N	1.91	0.81
1:E:274:ILE:HG23	1:E:306:ASN:HD21	1.41	0.81
2:N:261:VAL:HG13	2:N:276:VAL:HG21	1.61	0.81
1:M:277:ARG:NH1	1:M:336:GLN:HG3	1.94	0.81
1:E:221:HIS:HE1	1:E:228:LEU:HB2	1.45	0.81
1:M:485:ALA:O	1:M:489:SER:HB3	1.79	0.81
1:A:559:VAL:HG22	1:A:560:LEU:N	1.94	0.81
1:I:199:ARG:NH2	1:I:223:LYS:HB2	1.95	0.81
1:M:23:GLN:HE21	1:M:60:VAL:H	1.24	0.81
2:N:96:HIS:CE1	2:N:381:VAL:O	2.32	0.81
1:M:253:THR:HG22	1:M:292:VAL:HG22	1.62	0.81
1:A:274:ILE:HG23	1:A:306:ASN:HD21	1.45	0.81
1:E:24:TRP:HB2	1:E:25:PRO:HD2	1.62	0.80
1:I:485:ALA:O	1:I:489:SER:HB3	1.81	0.80
2:F:13:LYS:O	2:F:16:MET:HB2	1.81	0.80
1:I:503:LEU:O	1:I:507:GLN:HG3	1.81	0.80
1:I:100:LEU:HD21	1:I:181:TYR:CE1	2.17	0.80
1:M:73:LYS:HE3	1:M:146:TYR:OH	1.81	0.80
1:I:458:VAL:HG12	1:I:548:VAL:HG22	1.63	0.80
1:I:49:LYS:HE3	1:I:142:ILE:HD12	1.61	0.80
1:A:3:SER:OG	1:A:5:ILE:HG22	1.81	0.80
1:I:260:LEU:HD21	1:I:303:LEU:HD23	1.62	0.80
2:J:64:LYS:HE3	2:J:69:THR:HA	1.62	0.80
1:A:557:ARG:HD3	1:A:557:ARG:O	1.81	0.80
1:E:458:VAL:CG1	1:E:548:VAL:HG22	2.11	0.80
1:E:510:PRO:HB2	1:E:522:ILE:HD11	1.64	0.80
2:J:5:ILE:HD11	8:J:438:SWE:H4	1.64	0.80
2:J:281:LYS:O	2:J:284:ARG:HB2	1.81	0.80
2:F:314:VAL:HG22	2:F:315:HIS:N	1.97	0.80
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.43	0.79
1:A:221:HIS:H	1:A:221:HIS:CD2	1.96	0.79
1:E:500:GLN:HB3	2:F:422:LEU:HD13	1.63	0.79
2:N:421:PRO:HA	2:N:426:TRP:HE1	1.47	0.79
1:A:27:THR:O	1:A:31:ILE:HG13	1.82	0.79
2:N:13:LYS:O	2:N:16:MET:HB2	1.81	0.79
1:E:425:LEU:HD13	1:E:509:GLN:HE22	1.48	0.79
1:E:503:LEU:O	1:E:507:GLN:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:69:THR:HG22	2:N:69:THR:O	1.80	0.79
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.62	0.79
2:F:94:ILE:HD11	2:F:161:GLN:HG2	1.63	0.79
1:A:511:ASP:OD1	1:A:512:LYS:HG3	1.83	0.79
2:F:281:LYS:O	2:F:284:ARG:HB2	1.82	0.79
2:J:3:SER:N	2:J:4:PRO:HD3	1.98	0.79
1:E:278:GLN:HG3	1:E:298:GLU:HB3	1.64	0.79
2:B:281:LYS:O	2:B:284:ARG:HB2	1.83	0.79
1:I:458:VAL:CG1	1:I:548:VAL:HG22	2.13	0.78
1:E:103:LYS:HE3	1:E:179:VAL:HG21	1.64	0.78
4:H:821:DC:H2'	4:H:822:2DA:H8	1.63	0.78
1:E:441:TYR:HD1	1:E:544:GLY:HA3	1.43	0.78
2:J:30:LYS:HE2	2:J:62:ALA:O	1.81	0.78
2:B:194:GLU:OE2	2:B:195:ILE:HG22	1.84	0.78
2:F:171:PHE:HB2	2:F:208:HIS:ND1	1.99	0.78
2:F:314:VAL:HG22	2:F:315:HIS:H	1.48	0.77
1:A:503:LEU:O	1:A:507:GLN:HG3	1.84	0.77
1:M:163:SER:O	1:M:167:ILE:HD13	1.83	0.77
2:J:115:TYR:OH	2:J:157:PRO:HG3	1.84	0.77
1:M:155:GLY:O	1:M:159:ILE:HG12	1.83	0.77
2:B:314:VAL:HG22	2:B:315:HIS:N	2.00	0.77
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.66	0.77
1:E:52:PRO:HA	1:E:143:ARG:NH2	2.00	0.77
1:M:244:ILE:HD11	1:M:263:LYS:HG3	1.67	0.77
2:N:303:LEU:HD21	2:N:307:ARG:HH21	1.49	0.77
1:I:171:PHE:HB2	1:I:208:HIS:CD2	2.20	0.77
2:J:421:PRO:HA	2:J:426:TRP:HE1	1.49	0.77
2:B:94:ILE:HD11	2:B:161:GLN:HG2	1.66	0.77
1:E:235:HIS:HB2	1:E:238:LYS:O	1.85	0.77
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.66	0.76
2:F:421:PRO:HA	2:F:426:TRP:HE1	1.50	0.76
1:A:155:GLY:O	1:A:159:ILE:HG12	1.84	0.76
1:A:280:SER:O	1:A:283:LEU:HD12	1.85	0.76
2:J:303:LEU:HD21	2:J:307:ARG:HH21	1.49	0.76
1:E:73:LYS:HE3	1:E:146:TYR:OH	1.84	0.76
1:I:235:HIS:HB3	1:I:236:PRO:HD2	1.67	0.76
1:I:441:TYR:CE1	1:I:544:GLY:HA3	2.19	0.76
1:E:260:LEU:HD21	1:E:303:LEU:HD23	1.67	0.76
2:B:314:VAL:HG22	2:B:315:HIS:H	1.49	0.76
2:B:421:PRO:HA	2:B:426:TRP:HE1	1.49	0.76
2:J:314:VAL:HG22	2:J:315:HIS:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:SER:N	1:I:157:PRO:HD2	2.01	0.76
1:A:49:LYS:HE3	1:A:142:ILE:HD12	1.67	0.76
2:J:65:LYS:HA	2:J:407:GLN:HE21	1.51	0.76
1:E:221:HIS:CE1	1:E:228:LEU:H	2.04	0.76
1:E:3:SER:OG	1:E:5:ILE:HG22	1.84	0.76
2:N:65:LYS:HB2	2:N:68:SER:CB	2.15	0.76
1:I:23:GLN:HE21	1:I:60:VAL:H	1.33	0.76
1:A:27:THR:HB	1:A:30:LYS:HB2	1.67	0.76
1:M:548:VAL:O	1:M:552:VAL:HG22	1.86	0.75
2:J:314:VAL:HG22	2:J:315:HIS:N	2.01	0.75
1:M:278:GLN:HG3	1:M:298:GLU:HB3	1.68	0.75
1:E:463:ARG:HB2	1:E:463:ARG:NH1	2.02	0.75
1:E:463:ARG:HH11	1:E:463:ARG:HB2	1.51	0.75
3:C:709:DC:H2'	3:C:710:DG:H8	1.51	0.75
2:N:387:PRO:HG2	2:N:389:PHE:CE1	2.22	0.75
2:B:428:GLN:HG2	2:B:429:GLY:N	2.01	0.75
1:A:52:PRO:HA	1:A:143:ARG:NH2	2.01	0.75
4:H:817:MRG:H2'	4:H:818:DC:C6	2.21	0.75
2:F:254:VAL:HG13	2:F:283:LEU:HD22	1.68	0.74
1:E:102:LYS:HD2	1:E:102:LYS:N	2.01	0.74
1:E:548:VAL:O	1:E:552:VAL:HG22	1.86	0.74
2:J:100:LEU:H	2:J:100:LEU:HD23	1.52	0.74
1:I:511:ASP:OD1	1:I:512:LYS:HG2	1.84	0.74
1:E:211:ARG:HD2	2:J:5:ILE:HD13	1.67	0.74
1:A:72:ARG:HG3	1:A:151:GLN:HE22	1.50	0.74
1:I:24:TRP:HB2	1:I:25:PRO:HD2	1.68	0.74
1:E:27:THR:HB	1:E:30:LYS:HB2	1.69	0.74
2:N:281:LYS:O	2:N:284:ARG:HB2	1.87	0.74
2:B:33:ALA:O	2:B:37:ILE:HG12	1.88	0.74
1:E:221:HIS:H	1:E:221:HIS:CD2	2.05	0.74
2:F:303:LEU:HD21	2:F:307:ARG:HH21	1.50	0.74
2:N:314:VAL:HG22	2:N:315:HIS:N	2.02	0.74
1:I:207:GLN:NE2	1:I:210:LEU:HD23	2.01	0.74
1:I:463:ARG:HB2	1:I:463:ARG:HH11	1.52	0.74
1:I:463:ARG:HB2	1:I:463:ARG:NH1	2.02	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.74
2:B:64:LYS:CE	2:B:69:THR:HG23	2.18	0.74
2:F:194:GLU:OE2	2:F:195:ILE:HG22	1.87	0.74
2:N:314:VAL:HG22	2:N:315:HIS:H	1.52	0.74
2:J:387:PRO:HG2	2:J:389:PHE:CE1	2.23	0.74
1:E:447:ASN:HB2	1:E:556:ILE:HG23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:HD11	1:E:263:LYS:HG3	1.70	0.74
2:J:33:ALA:O	2:J:37:ILE:HG12	1.88	0.74
1:I:510:PRO:HB2	1:I:522:ILE:HD11	1.70	0.74
1:I:228:LEU:HA	1:I:232:TYR:O	1.88	0.74
1:I:425:LEU:HD13	1:I:509:GLN:HE22	1.51	0.74
2:J:254:VAL:HG13	2:J:283:LEU:HD22	1.69	0.74
4:P:805:DG:H5''	9:P:81:HOH:O	1.88	0.74
1:M:511:ASP:OD1	1:M:512:LYS:CG	2.36	0.73
1:A:73:LYS:O	1:A:74:LEU:HD23	1.88	0.73
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.70	0.73
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.70	0.73
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.68	0.73
2:B:64:LYS:HE3	2:B:69:THR:CA	2.14	0.73
1:A:73:LYS:HE3	1:A:146:TYR:OH	1.88	0.73
1:I:101:LYS:CE	1:I:321:PRO:HG3	2.17	0.73
2:B:369:THR:O	2:B:373:GLN:HG3	1.88	0.73
2:N:100:LEU:H	2:N:100:LEU:HD23	1.53	0.73
1:A:425:LEU:HD13	1:A:509:GLN:HE22	1.53	0.73
1:A:156:SER:N	1:A:157:PRO:HD2	2.03	0.73
2:J:234:LEU:N	2:J:234:LEU:HD12	2.03	0.73
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.69	0.73
1:M:510:PRO:HB2	1:M:522:ILE:HD11	1.71	0.73
1:I:229:TRP:CE2	1:I:230:MET:HG2	2.24	0.73
2:N:33:ALA:O	2:N:37:ILE:HG12	1.89	0.73
1:M:90:VAL:CG2	2:N:140:PRO:HB2	2.17	0.72
2:F:387:PRO:HG2	2:F:389:PHE:CE1	2.24	0.72
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.24	0.72
1:E:171:PHE:HB2	1:E:208:HIS:CD2	2.24	0.72
2:B:74:LEU:HD12	2:B:75:VAL:N	2.04	0.72
3:C:708:DG:H2'	3:C:709:DC:C6	2.25	0.72
2:B:94:ILE:CD1	2:B:161:GLN:HG2	2.19	0.72
1:A:163:SER:O	1:A:167:ILE:HD13	1.88	0.72
1:A:320:ASP:OD2	1:A:323:LYS:HE2	1.89	0.72
1:E:511:ASP:OD1	1:E:512:LYS:CG	2.35	0.72
2:J:115:TYR:CZ	2:J:157:PRO:HG3	2.24	0.72
1:I:101:LYS:HE3	1:I:321:PRO:CG	2.19	0.72
1:I:90:VAL:HG23	2:J:141:GLY:O	1.88	0.72
2:F:33:ALA:O	2:F:37:ILE:HG12	1.90	0.71
1:M:108:VAL:O	1:M:220:LYS:HB2	1.89	0.71
2:F:94:ILE:CD1	2:F:161:GLN:HG2	2.20	0.71
1:I:27:THR:O	1:I:31:ILE:HG13	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:ILE:HD11	1:I:263:LYS:HG3	1.71	0.71
1:I:286:THR:O	1:I:287:LYS:CG	2.32	0.71
3:K:709:DC:H2'	3:K:710:DG:H8	1.55	0.71
2:F:74:LEU:HD12	2:F:75:VAL:N	2.05	0.71
1:A:221:HIS:H	1:A:221:HIS:HD2	1.38	0.71
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.71	0.71
1:E:27:THR:O	1:E:31:ILE:HG13	1.90	0.71
1:M:156:SER:N	1:M:157:PRO:HD2	2.05	0.71
2:N:115:TYR:CZ	2:N:157:PRO:HG3	2.26	0.71
1:M:116:PHE:HA	1:M:148:VAL:HG21	1.73	0.71
2:N:194:GLU:OE2	2:N:195:ILE:HG22	1.90	0.71
1:M:4:PRO:HD2	1:M:212:TRP:O	1.90	0.71
1:I:199:ARG:O	1:I:203:GLU:HG2	1.91	0.71
1:I:100:LEU:CD2	1:I:181:TYR:CE1	2.74	0.71
1:A:533:LEU:N	1:A:533:LEU:HD12	2.06	0.71
4:D:817:MRG:H2'	4:D:818:DC:C6	2.26	0.71
2:N:62:ALA:O	2:N:63:ILE:CG2	2.39	0.70
1:I:2:ILE:H	1:I:2:ILE:HD12	1.55	0.70
1:A:548:VAL:O	1:A:552:VAL:HG22	1.90	0.70
2:F:175:ASN:HD21	2:F:201:LYS:NZ	1.90	0.70
2:B:122:GLU:HA	2:B:125:ARG:HE	1.57	0.70
1:E:277:ARG:NH1	1:E:336:GLN:CG	2.54	0.70
1:I:223:LYS:HG3	1:I:223:LYS:O	1.90	0.70
2:N:244:ILE:HD13	2:N:244:ILE:H	1.55	0.70
1:I:469:LEU:HD21	1:I:480:GLN:HG3	1.73	0.70
2:F:64:LYS:CE	2:F:69:THR:HG23	2.22	0.70
2:J:37:ILE:O	2:J:41:MET:HG3	1.90	0.70
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.73	0.70
2:J:372:VAL:HG13	2:J:389:PHE:CE2	2.26	0.70
2:F:376:THR:O	2:F:380:ILE:HG13	1.91	0.70
1:M:260:LEU:HD21	1:M:303:LEU:HD23	1.73	0.70
1:I:91:GLN:HG3	1:I:161:GLN:HE22	1.56	0.70
1:E:221:HIS:CE1	1:E:228:LEU:HB2	2.25	0.70
1:I:329:ILE:HD11	1:I:375:ILE:HD12	1.72	0.70
4:L:821:DC:H2'	4:L:822:2DA:H8	1.73	0.70
1:I:439:THR:CG2	2:J:289:LEU:HD13	2.20	0.70
1:A:23:GLN:HE21	1:A:60:VAL:H	1.38	0.70
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.27	0.70
2:J:72:ARG:HH21	2:J:409:THR:HG22	1.55	0.70
2:N:254:VAL:HG13	2:N:283:LEU:HD22	1.72	0.70
1:I:253:THR:HG22	1:I:292:VAL:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:LEU:H	2:F:100:LEU:CD2	2.04	0.69
1:I:548:VAL:O	1:I:552:VAL:HG22	1.92	0.69
3:G:723:DC:H2''	3:G:724:DT:O5'	1.92	0.69
1:E:23:GLN:HE21	1:E:60:VAL:H	1.40	0.69
4:P:821:DC:H2'	4:P:822:2DA:H8	1.72	0.69
1:I:101:LYS:HE3	1:I:321:PRO:HG3	1.73	0.69
1:I:278:GLN:HG3	1:I:298:GLU:HB3	1.74	0.69
2:N:47:ILE:HG22	2:N:146:TYR:HA	1.74	0.69
1:I:435:VAL:CA	2:J:290:THR:HG21	2.23	0.69
2:F:372:VAL:HG13	2:F:389:PHE:CE2	2.26	0.69
1:E:280:SER:O	1:E:283:LEU:HD12	1.92	0.69
1:I:303:LEU:O	1:I:307:ARG:HB2	1.93	0.69
1:M:458:VAL:HG13	1:M:548:VAL:HG22	1.73	0.69
1:E:394:GLN:HB2	1:E:397:THR:OG1	1.92	0.69
1:I:451:LYS:O	1:I:471:ASN:HA	1.92	0.69
1:E:277:ARG:HH11	1:E:336:GLN:HG3	1.54	0.69
1:I:558:LYS:HE3	1:I:559:VAL:O	1.92	0.69
1:I:238:LYS:HZ1	1:I:347:LYS:HE2	1.57	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.91	0.69
1:I:441:TYR:CD1	1:I:544:GLY:CA	2.63	0.69
1:M:27:THR:O	1:M:31:ILE:HG13	1.92	0.69
1:E:451:LYS:O	1:E:471:ASN:HA	1.93	0.69
2:B:303:LEU:HD21	2:B:307:ARG:HH21	1.56	0.69
1:E:65:LYS:NZ	1:E:70:ARG:HH21	1.90	0.69
1:M:451:LYS:O	1:M:471:ASN:HA	1.93	0.69
1:M:288:ALA:HB3	1:M:291:GLU:HG3	1.75	0.69
4:P:802:DA:H4'	4:P:803:DC:OP1	1.93	0.69
2:N:156:SER:HB2	2:N:157:PRO:HD3	1.74	0.69
2:J:194:GLU:OE2	2:J:195:ILE:HG22	1.91	0.69
2:J:94:ILE:HD11	2:J:161:GLN:HG2	1.75	0.69
2:J:243:PRO:HB2	2:J:244:ILE:HD13	1.75	0.69
1:I:101:LYS:HE3	1:I:321:PRO:HD3	1.75	0.69
2:N:371:ALA:O	2:N:375:ILE:HG12	1.92	0.69
2:F:234:LEU:HD12	2:F:234:LEU:N	2.08	0.69
1:M:469:LEU:HD21	1:M:480:GLN:HG3	1.75	0.68
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.27	0.68
2:N:78:ARG:HD3	2:N:411:ILE:HB	1.76	0.68
1:M:329:ILE:HD11	1:M:375:ILE:HD12	1.74	0.68
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.74	0.68
1:E:469:LEU:HD21	1:E:480:GLN:HG3	1.75	0.68
1:M:303:LEU:O	1:M:307:ARG:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:709:DC:H2'	3:G:710:DG:H8	1.59	0.68
2:F:100:LEU:HD23	2:F:100:LEU:N	2.08	0.68
1:E:3:SER:HB3	1:E:119:PRO:HD3	1.73	0.68
1:E:366:LYS:O	1:E:370:GLU:HG3	1.92	0.68
1:A:135:ILE:HD12	1:A:135:ILE:N	2.09	0.68
2:F:356:ARG:HG2	2:F:357:MET:H	1.59	0.68
2:F:37:ILE:O	2:F:41:MET:HG3	1.93	0.68
2:N:31:ILE:O	2:N:35:VAL:HG23	1.94	0.68
2:J:376:THR:HG23	2:J:386:THR:HG23	1.74	0.68
1:E:171:PHE:HB2	1:E:208:HIS:HD2	1.59	0.68
2:N:369:THR:O	2:N:373:GLN:HG3	1.94	0.68
2:J:371:ALA:O	2:J:375:ILE:HG12	1.92	0.68
2:N:122:GLU:HA	2:N:125:ARG:HE	1.59	0.68
1:A:237:ASP:OD2	1:A:238:LYS:HD3	1.94	0.68
1:I:209:LEU:HB3	1:I:214:LEU:HB2	1.74	0.68
2:B:100:LEU:H	2:B:100:LEU:CD2	2.06	0.68
1:M:209:LEU:HB3	1:M:214:LEU:HB2	1.76	0.68
2:F:376:THR:HG23	2:F:386:THR:HG23	1.75	0.67
4:P:818:DC:H2'	4:P:819:DG:H8	1.59	0.67
1:A:102:LYS:HD2	1:A:102:LYS:N	2.05	0.67
3:G:708:DG:H2'	3:G:709:DC:C6	2.29	0.67
3:C:709:DC:H2'	3:C:710:DG:C8	2.28	0.67
1:A:235:HIS:HB2	1:A:238:LYS:O	1.94	0.67
4:P:818:DC:H2'	4:P:819:DG:C8	2.29	0.67
1:A:90:VAL:HG22	2:B:140:PRO:HB2	1.75	0.67
2:B:376:THR:O	2:B:380:ILE:HG13	1.94	0.67
1:I:103:LYS:HE3	1:I:179:VAL:CG2	2.23	0.67
1:E:148:VAL:O	1:E:150:PRO:HD3	1.94	0.67
2:J:31:ILE:O	2:J:35:VAL:HG23	1.94	0.67
1:E:132:ILE:O	1:E:141:GLY:HA3	1.94	0.67
2:N:376:THR:HG23	2:N:386:THR:HG23	1.76	0.67
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.76	0.67
4:L:818:DC:H2'	4:L:819:DG:C8	2.29	0.67
1:E:317:VAL:HG11	1:E:347:LYS:HB3	1.75	0.67
2:N:184:MET:SD	2:N:410:TRP:HB3	2.35	0.67
4:L:818:DC:H2'	4:L:819:DG:H8	1.59	0.67
1:A:70:ARG:HH12	6:A:823:ZP4:C31	2.07	0.67
1:A:221:HIS:CD2	1:A:221:HIS:N	2.62	0.67
1:M:94:ILE:HD11	3:O:708:DG:H21	1.60	0.67
1:M:425:LEU:HD13	1:M:509:GLN:HE22	1.59	0.67
1:E:329:ILE:HD11	1:E:375:ILE:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:PHE:HB2	1:E:234:LEU:HB2	1.76	0.67
2:F:64:LYS:HE3	2:F:69:THR:CA	2.20	0.67
3:G:705:DA:H2''	3:G:706:DT:O5'	1.94	0.67
1:A:135:ILE:H	1:A:135:ILE:CD1	2.08	0.67
1:E:303:LEU:O	1:E:307:ARG:HB2	1.94	0.67
2:J:156:SER:HB2	2:J:157:PRO:HD3	1.76	0.67
1:E:277:ARG:HH11	1:E:336:GLN:CG	2.08	0.67
1:A:559:VAL:HG22	1:A:560:LEU:H	1.58	0.67
2:J:107:THR:HG23	2:J:232:TYR:HE2	1.58	0.67
1:A:451:LYS:O	1:A:471:ASN:HA	1.95	0.67
1:E:136:ASN:OD1	1:E:138:GLU:HG3	1.95	0.67
1:A:148:VAL:O	1:A:150:PRO:HD3	1.95	0.67
1:M:184:MET:HG3	4:P:822:2DA:H2'	1.75	0.66
2:J:72:ARG:HH22	2:J:151:GLN:HB3	1.60	0.66
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.77	0.66
1:I:280:SER:O	1:I:283:LEU:HD12	1.94	0.66
4:D:802:DA:H4'	4:D:803:DC:OP1	1.93	0.66
1:A:518:VAL:O	1:A:522:ILE:HG12	1.94	0.66
1:M:556:ILE:HG13	1:M:557:ARG:N	2.10	0.66
1:E:22:LYS:HG2	1:E:23:GLN:N	2.10	0.66
1:M:135:ILE:N	1:M:135:ILE:HD12	2.08	0.66
2:F:75:VAL:HG11	2:F:77:PHE:CE2	2.31	0.66
1:A:559:VAL:CG2	1:A:560:LEU:N	2.58	0.66
1:E:463:ARG:CB	1:E:463:ARG:HH11	2.08	0.66
2:J:66:LYS:O	2:J:67:ASP:HB2	1.94	0.66
2:J:125:ARG:HG2	2:J:146:TYR:O	1.96	0.66
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.76	0.66
1:E:435:VAL:HA	2:F:290:THR:HG21	1.75	0.66
1:M:135:ILE:CD1	1:M:135:ILE:H	2.08	0.66
1:I:195:ILE:O	1:I:199:ARG:HG2	1.96	0.66
2:F:369:THR:O	2:F:373:GLN:HG3	1.96	0.66
2:B:371:ALA:O	2:B:375:ILE:HG12	1.96	0.66
1:I:394:GLN:HB2	1:I:397:THR:OG1	1.95	0.66
2:J:369:THR:O	2:J:373:GLN:HG3	1.96	0.66
2:J:6:GLU:HA	2:J:6:GLU:OE1	1.95	0.66
2:N:171:PHE:HB2	2:N:208:HIS:CE1	2.31	0.66
2:F:314:VAL:CG2	2:F:315:HIS:H	2.08	0.66
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.31	0.66
2:J:403:THR:HG23	9:J:449:HOH:O	1.95	0.66
1:M:116:PHE:HA	1:M:148:VAL:CG2	2.26	0.66
2:N:372:VAL:HG13	2:N:389:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:72:ARG:NH1	2:N:151:GLN:OE1	2.26	0.66
2:J:376:THR:O	2:J:380:ILE:HG13	1.96	0.65
2:B:100:LEU:HD23	2:B:100:LEU:N	2.11	0.65
1:A:559:VAL:CG2	1:A:560:LEU:H	2.09	0.65
2:F:418:ASN:O	2:F:419:THR:HG23	1.95	0.65
1:M:53:GLU:O	1:M:55:PRO:HD3	1.96	0.65
1:M:195:ILE:O	1:M:199:ARG:HG2	1.96	0.65
4:D:818:DC:H2'	4:D:819:DG:C8	2.31	0.65
2:N:78:ARG:HA	2:N:81:ASN:HD22	1.60	0.65
1:E:557:ARG:O	1:E:558:LYS:HG2	1.96	0.65
2:B:247:PRO:HA	2:B:431:HIS:CA	2.26	0.65
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.79	0.65
1:M:408:ALA:HB3	2:N:393:ILE:HB	1.78	0.65
1:A:303:LEU:O	1:A:307:ARG:HB2	1.96	0.65
1:M:394:GLN:HB2	1:M:397:THR:OG1	1.96	0.65
2:F:261:VAL:HG13	2:F:276:VAL:CG2	2.25	0.65
1:I:238:LYS:NZ	1:I:347:LYS:HE2	2.12	0.65
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.78	0.65
1:M:26:LEU:HD12	1:M:133:PRO:HG3	1.78	0.65
2:F:50:ILE:HG21	2:F:145:GLN:OE1	1.95	0.65
2:J:234:LEU:H	2:J:234:LEU:CD1	2.09	0.65
3:K:709:DC:H2'	3:K:710:DG:C8	2.32	0.65
2:F:175:ASN:HD21	2:F:201:LYS:CE	2.09	0.65
3:O:707:DG:H2''	3:O:708:DG:H5'	1.78	0.65
2:B:314:VAL:CG2	2:B:315:HIS:H	2.08	0.65
2:F:356:ARG:HG2	2:F:357:MET:N	2.12	0.65
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.26	0.65
1:I:324:ASP:HA	1:I:385:LYS:HZ1	1.62	0.65
1:A:557:ARG:O	1:A:557:ARG:CD	2.44	0.65
2:F:319:TYR:OH	2:F:385:LYS:HD3	1.97	0.65
3:G:709:DC:H2'	3:G:710:DG:C8	2.32	0.65
1:M:70:ARG:HG2	1:M:71:TRP:H	1.59	0.65
2:J:314:VAL:CG2	2:J:315:HIS:H	2.10	0.65
2:N:37:ILE:O	2:N:41:MET:HG3	1.96	0.65
1:E:181:TYR:CE1	2:F:138:GLU:HG2	2.32	0.65
1:M:207:GLN:NE2	1:M:210:LEU:HD23	2.12	0.65
2:F:69:THR:O	2:F:69:THR:HG22	1.97	0.64
3:G:707:DG:H2''	3:G:708:DG:H5'	1.79	0.64
1:E:518:VAL:O	1:E:522:ILE:HG12	1.96	0.64
1:E:425:LEU:HD13	1:E:509:GLN:NE2	2.12	0.64
2:J:78:ARG:HA	2:J:81:ASN:HD22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:VAL:HB	1:I:149:LEU:HD22	1.79	0.64
1:M:130:PHE:CZ	1:M:144:TYR:HB2	2.32	0.64
1:M:27:THR:HB	1:M:30:LYS:HB2	1.78	0.64
1:A:277:ARG:HH11	1:A:336:GLN:HG3	1.60	0.64
2:J:171:PHE:HB2	2:J:208:HIS:CE1	2.33	0.64
2:F:78:ARG:HA	2:F:81:ASN:HD22	1.62	0.64
2:J:169:GLU:HA	2:J:169:GLU:OE2	1.97	0.64
3:C:723:DC:H2''	3:C:724:DT:O5'	1.96	0.64
2:J:175:ASN:HD21	2:J:201:LYS:NZ	1.95	0.64
1:M:439:THR:CG2	2:N:289:LEU:HD13	2.26	0.64
2:N:72:ARG:HH22	2:N:151:GLN:HB3	1.62	0.64
1:I:320:ASP:OD2	1:I:323:LYS:HE2	1.97	0.64
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.78	0.64
1:E:135:ILE:HD12	1:E:135:ILE:N	2.13	0.64
2:N:8:VAL:HG21	2:N:159:ILE:HD12	1.79	0.64
1:M:227:PHE:HB2	1:M:234:LEU:HB2	1.80	0.64
1:A:217:PRO:HB2	1:A:219:GLN:NE2	2.11	0.64
1:M:24:TRP:HB2	1:M:25:PRO:HD2	1.79	0.64
2:F:371:ALA:O	2:F:375:ILE:HG12	1.97	0.64
1:I:199:ARG:HH22	1:I:223:LYS:HB2	1.60	0.64
1:E:463:ARG:HG2	1:E:464:GLN:N	2.13	0.64
1:E:556:ILE:HD12	1:E:556:ILE:N	2.12	0.64
1:M:447:ASN:HA	1:M:556:ILE:HD13	1.80	0.64
4:D:821:DC:H2'	4:D:822:2DA:H8	1.78	0.64
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.33	0.64
2:B:64:LYS:CE	2:B:69:THR:HA	2.17	0.64
2:J:115:TYR:HB3	2:J:149:LEU:HB2	1.78	0.64
1:M:73:LYS:HE3	1:M:146:TYR:CZ	2.32	0.64
1:I:463:ARG:CB	1:I:463:ARG:HH11	2.10	0.64
1:I:229:TRP:NE1	1:I:230:MET:HG2	2.13	0.64
1:E:301:LEU:O	1:E:304:ALA:HB3	1.98	0.64
1:E:441:TYR:CE1	1:E:544:GLY:HA3	2.30	0.64
1:E:207:GLN:HE22	1:E:210:LEU:HD23	1.63	0.64
1:M:46:LYS:HD3	1:M:116:PHE:HB3	1.79	0.64
1:M:529:GLU:O	1:M:530:LYS:HG3	1.97	0.64
1:I:130:PHE:CZ	1:I:144:TYR:HB2	2.33	0.64
1:E:163:SER:O	1:E:167:ILE:HD13	1.96	0.64
2:B:125:ARG:HG2	2:B:146:TYR:O	1.98	0.64
2:N:418:ASN:O	2:N:419:THR:HG23	1.97	0.64
1:I:90:VAL:HG22	2:J:140:PRO:HB2	1.79	0.64
3:K:723:DC:H2''	3:K:724:DT:O5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:153:TRP:CZ2	2:N:155:GLY:HA3	2.33	0.64
2:B:69:THR:HG22	2:B:69:THR:O	1.96	0.64
2:J:118:VAL:HG22	8:J:438:SWE:H3	1.80	0.64
2:F:28:GLU:HA	2:F:135:ILE:HD11	1.80	0.64
1:E:64:LYS:HD3	1:E:68:SER:HB3	1.79	0.64
1:I:109:LEU:HG	1:I:220:LYS:HD2	1.79	0.64
3:O:709:DC:H2'	3:O:710:DG:H8	1.62	0.63
2:J:100:LEU:H	2:J:100:LEU:CD2	2.10	0.63
2:J:195:ILE:HG13	2:J:199:ARG:NH1	2.13	0.63
1:A:394:GLN:HB2	1:A:397:THR:OG1	1.98	0.63
1:A:324:ASP:HA	1:A:385:LYS:HZ1	1.63	0.63
2:F:7:THR:HG22	2:F:119:PRO:HG2	1.80	0.63
1:I:132:ILE:O	1:I:141:GLY:HA3	1.98	0.63
2:J:122:GLU:HA	2:J:125:ARG:HE	1.63	0.63
2:N:13:LYS:HD3	2:N:86:ASP:HB2	1.80	0.63
2:N:153:TRP:CE2	2:N:155:GLY:HA3	2.33	0.63
1:I:442:VAL:HG11	1:I:485:ALA:HB2	1.80	0.63
2:B:64:LYS:HE2	2:B:69:THR:HG23	1.78	0.63
1:E:27:THR:HB	1:E:30:LYS:CB	2.28	0.63
2:F:31:ILE:O	2:F:35:VAL:HG23	1.97	0.63
1:M:366:LYS:O	1:M:370:GLU:HG3	1.97	0.63
1:E:209:LEU:HB3	1:E:214:LEU:HB2	1.79	0.63
1:E:255:ASN:HD22	1:E:289:LEU:HD22	1.63	0.63
1:A:221:HIS:CE1	1:A:228:LEU:HB2	2.28	0.63
3:C:707:DG:H2'	3:C:708:DG:H8	1.63	0.63
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.33	0.63
2:F:241:VAL:HG13	2:F:351:THR:N	2.13	0.63
1:A:109:LEU:N	1:A:109:LEU:HD12	2.14	0.63
1:I:277:ARG:HH11	1:I:336:GLN:HG3	1.61	0.63
1:A:425:LEU:HD13	1:A:509:GLN:NE2	2.13	0.63
2:B:31:ILE:O	2:B:35:VAL:HG23	1.98	0.63
1:I:324:ASP:HA	1:I:385:LYS:NZ	2.13	0.63
1:E:195:ILE:O	1:E:199:ARG:HG2	1.97	0.63
2:N:175:ASN:HD21	2:N:201:LYS:NZ	1.97	0.63
2:N:377:THR:HA	2:N:380:ILE:HD12	1.80	0.63
1:I:500:GLN:HB3	2:J:422:LEU:HD13	1.80	0.63
1:I:3:SER:OG	1:I:5:ILE:HG22	1.99	0.63
2:J:60:VAL:CG1	2:J:75:VAL:HG22	2.29	0.63
2:J:13:LYS:HD3	2:J:86:ASP:HB2	1.79	0.63
4:D:818:DC:H2'	4:D:819:DG:H8	1.64	0.63
1:M:49:LYS:HE3	1:M:142:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:91:GLN:HG3	1:M:161:GLN:HE22	1.63	0.62
2:N:303:LEU:HD21	2:N:307:ARG:NH2	2.14	0.62
1:E:73:LYS:NZ	1:E:130:PHE:CE2	2.60	0.62
1:M:132:ILE:O	1:M:141:GLY:HA3	1.99	0.62
1:M:67:ASN:O	1:M:68:SER:CB	2.44	0.62
2:B:418:ASN:O	2:B:419:THR:HG23	1.99	0.62
2:N:100:LEU:H	2:N:100:LEU:CD2	2.11	0.62
2:B:339:TYR:CD2	2:B:375:ILE:HD12	2.33	0.62
1:A:22:LYS:HG2	1:A:23:GLN:N	2.14	0.62
2:J:244:ILE:CD1	2:J:244:ILE:H	2.12	0.62
2:J:303:LEU:HD21	2:J:307:ARG:NH2	2.14	0.62
2:N:314:VAL:CG2	2:N:315:HIS:H	2.13	0.62
3:K:706:DT:H2'	3:K:707:DG:C8	2.34	0.62
1:A:237:ASP:O	1:A:238:LYS:HD2	1.99	0.62
1:I:136:ASN:HB3	1:I:138:GLU:HG3	1.81	0.62
1:I:529:GLU:O	1:I:530:LYS:HG3	1.99	0.62
2:J:153:TRP:CZ2	2:J:155:GLY:HA3	2.34	0.62
2:N:6:GLU:HA	2:N:6:GLU:OE1	1.99	0.62
2:F:244:ILE:H	2:F:244:ILE:CD1	2.12	0.62
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.14	0.62
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.81	0.62
1:E:398:TRP:CZ2	1:E:411:ILE:HG12	2.34	0.62
1:I:49:LYS:CE	1:I:142:ILE:HD12	2.28	0.62
1:A:132:ILE:O	1:A:141:GLY:HA3	1.99	0.62
1:A:15:GLY:HA2	2:F:165:THR:HG21	1.82	0.62
1:A:301:LEU:O	1:A:304:ALA:HB3	2.00	0.62
2:F:122:GLU:HA	2:F:125:ARG:HE	1.65	0.62
2:J:149:LEU:HB3	2:J:156:SER:OG	1.99	0.62
2:N:74:LEU:HD12	2:N:75:VAL:N	2.15	0.62
1:E:135:ILE:CD1	1:E:135:ILE:H	2.12	0.62
1:I:31:ILE:O	1:I:35:VAL:HG23	1.98	0.62
4:L:802:DA:H4'	4:L:803:DC:OP1	2.00	0.62
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.00	0.62
2:J:47:ILE:HG22	2:J:146:TYR:HA	1.80	0.62
1:M:94:ILE:CD1	3:O:708:DG:H21	2.12	0.62
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.47	0.62
2:F:241:VAL:HG13	2:F:351:THR:H	1.65	0.62
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.98	0.62
2:J:418:ASN:O	2:J:419:THR:HG23	1.99	0.62
3:G:706:DT:H2'	3:G:707:DG:H8	1.64	0.62
2:F:153:TRP:CE2	2:F:155:GLY:HA3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:ILE:HG23	2:F:6:GLU:N	2.15	0.62
1:I:285:GLY:N	3:K:714:DG:OP1	2.32	0.62
1:M:442:VAL:HB	1:M:481:ALA:HB1	1.81	0.62
4:H:818:DC:H2'	4:H:819:DG:C8	2.35	0.62
2:J:74:LEU:HD12	2:J:75:VAL:N	2.15	0.62
2:N:69:THR:CG2	2:N:69:THR:O	2.47	0.62
1:E:164:MET:HE2	1:E:168:LEU:HD11	1.82	0.62
2:F:303:LEU:HD21	2:F:307:ARG:NH2	2.14	0.62
2:B:303:LEU:HD23	2:B:303:LEU:C	2.19	0.62
1:A:324:ASP:HA	1:A:385:LYS:NZ	2.15	0.62
2:F:31:ILE:CD1	2:F:133:PRO:HG2	2.30	0.62
2:J:5:ILE:CG1	2:J:6:GLU:H	2.08	0.61
1:E:118:VAL:O	1:E:148:VAL:HG23	2.00	0.61
1:E:438:GLU:OE2	1:E:463:ARG:NH1	2.33	0.61
1:I:101:LYS:HE3	1:I:321:PRO:CD	2.29	0.61
3:K:707:DG:H2''	3:K:708:DG:H5'	1.80	0.61
1:E:253:THR:HG22	1:E:292:VAL:HG22	1.81	0.61
2:N:125:ARG:HG2	2:N:146:TYR:O	2.00	0.61
2:J:24:TRP:CH2	2:J:403:THR:HG21	2.35	0.61
1:A:103:LYS:HE3	1:A:179:VAL:CG2	2.28	0.61
1:A:116:PHE:C	1:A:148:VAL:HG21	2.21	0.61
2:F:303:LEU:C	2:F:303:LEU:HD23	2.20	0.61
1:E:446:ALA:C	1:E:556:ILE:HG21	2.21	0.61
1:A:329:ILE:HG12	1:A:339:TYR:HB3	1.82	0.61
1:M:320:ASP:OD2	1:M:323:LYS:HE2	1.99	0.61
1:A:194:GLU:HA	1:A:194:GLU:OE1	1.99	0.61
1:A:195:ILE:O	1:A:199:ARG:HG2	1.99	0.61
2:J:111:VAL:HG11	2:J:187:LEU:HD22	1.81	0.61
1:E:303:LEU:HD13	1:E:303:LEU:O	2.01	0.61
2:F:314:VAL:CG2	2:F:315:HIS:N	2.63	0.61
2:N:24:TRP:CZ3	2:N:403:THR:HG21	2.36	0.61
1:I:274:ILE:HG23	1:I:306:ASN:ND2	2.07	0.61
1:E:27:THR:HG22	1:E:30:LYS:H	1.66	0.61
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.82	0.61
1:I:366:LYS:O	1:I:370:GLU:HG3	2.00	0.61
2:F:156:SER:HB2	2:F:157:PRO:HD3	1.80	0.61
1:A:74:LEU:HD13	3:C:705:DA:C5	2.34	0.61
1:E:31:ILE:O	1:E:35:VAL:HG23	2.00	0.61
1:I:463:ARG:HG2	1:I:464:GLN:N	2.16	0.61
1:I:425:LEU:HD13	1:I:509:GLN:NE2	2.15	0.61
1:A:64:LYS:HE3	1:A:71:TRP:CZ2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ILE:O	2:F:136:ASN:HB2	2.01	0.61
2:B:195:ILE:HG13	2:B:199:ARG:NH1	2.15	0.61
1:M:76:ASP:OD1	3:O:705:DA:H4'	2.00	0.61
2:F:426:TRP:HD1	2:F:426:TRP:H	1.48	0.61
1:E:463:ARG:HG2	1:E:464:GLN:H	1.64	0.61
1:A:543:GLY:HA2	2:B:283:LEU:O	2.00	0.61
2:B:101:LYS:HG2	2:B:102:LYS:HG3	1.82	0.61
1:A:438:GLU:OE2	1:A:463:ARG:NH1	2.33	0.61
1:E:288:ALA:HB3	1:E:291:GLU:HG3	1.82	0.61
1:E:408:ALA:HB3	2:F:393:ILE:HB	1.83	0.61
3:O:709:DC:H2'	3:O:710:DG:C8	2.36	0.61
1:I:31:ILE:HG23	1:I:133:PRO:HG2	1.83	0.61
2:J:336:GLN:NE2	2:J:353:LYS:HD3	2.16	0.61
1:I:277:ARG:NH1	1:I:336:GLN:CG	2.63	0.61
2:B:376:THR:HG23	2:B:386:THR:HG23	1.82	0.61
2:F:26:LEU:HD12	2:F:31:ILE:HD13	1.82	0.61
2:B:78:ARG:HA	2:B:81:ASN:HD22	1.65	0.61
1:M:438:GLU:HG2	1:M:461:LYS:HD3	1.83	0.61
1:I:398:TRP:CZ2	1:I:411:ILE:HG12	2.36	0.61
1:A:435:VAL:HA	2:B:290:THR:HG21	1.81	0.61
1:A:27:THR:HB	1:A:30:LYS:CB	2.30	0.61
1:M:235:HIS:HB2	1:M:238:LYS:O	2.01	0.61
1:I:77:PHE:HB2	1:I:152:GLY:O	2.01	0.61
1:A:437:ALA:HB1	1:A:492:GLU:O	2.01	0.61
3:G:706:DT:H2'	3:G:707:DG:C8	2.36	0.60
1:I:155:GLY:O	1:I:159:ILE:CG1	2.49	0.60
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.35	0.60
1:M:115:TYR:CE2	6:M:823:ZP4:H2'A	2.36	0.60
2:N:244:ILE:N	2:N:244:ILE:HD13	2.15	0.60
1:E:90:VAL:HG22	2:F:140:PRO:HB2	1.83	0.60
1:I:447:ASN:HB3	1:I:450:THR:OG1	2.00	0.60
2:B:171:PHE:H	2:B:208:HIS:HE1	1.49	0.60
2:J:153:TRP:CE2	2:J:155:GLY:HA3	2.36	0.60
2:N:60:VAL:CG1	2:N:75:VAL:HG22	2.28	0.60
1:M:115:TYR:CD2	6:M:823:ZP4:H2'A	2.36	0.60
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.14	0.60
1:A:438:GLU:HG2	1:A:461:LYS:HD3	1.83	0.60
1:E:46:LYS:O	1:E:147:ASN:HB2	2.01	0.60
1:I:239:TRP:CE2	1:I:316:GLY:HA3	2.36	0.60
3:O:707:DG:H2'	3:O:708:DG:H8	1.66	0.60
2:F:195:ILE:HG13	2:F:199:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:518:VAL:O	1:M:522:ILE:HG12	2.02	0.60
3:K:706:DT:H2'	3:K:707:DG:H8	1.66	0.60
2:N:26:LEU:HD12	2:N:31:ILE:HD13	1.83	0.60
1:A:52:PRO:HG2	2:F:318:TYR:CD1	2.35	0.60
1:M:27:THR:HB	1:M:30:LYS:CB	2.32	0.60
2:N:64:LYS:HE3	2:N:69:THR:CA	2.31	0.60
1:A:221:HIS:CE1	1:A:228:LEU:H	2.19	0.60
2:N:62:ALA:O	2:N:63:ILE:HG23	2.01	0.60
2:B:356:ARG:HG2	2:B:357:MET:H	1.67	0.60
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.67	0.60
1:I:221:HIS:H	1:I:221:HIS:CD2	2.20	0.60
1:I:53:GLU:O	1:I:55:PRO:HD3	2.01	0.60
1:I:67:ASN:O	1:I:68:SER:CB	2.46	0.60
3:C:706:DT:H2'	3:C:707:DG:C8	2.36	0.60
1:I:463:ARG:HG2	1:I:464:GLN:H	1.67	0.60
1:E:339:TYR:CD1	1:E:375:ILE:HD11	2.37	0.60
1:M:238:LYS:HG2	1:M:315:HIS:ND1	2.15	0.60
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.16	0.60
2:N:64:LYS:NZ	2:N:69:THR:O	2.30	0.60
1:M:2:ILE:HD11	1:M:45:GLY:O	2.02	0.60
2:B:314:VAL:CG2	2:B:315:HIS:N	2.65	0.60
1:A:109:LEU:HA	1:A:220:LYS:HB2	1.84	0.60
2:J:428:GLN:HG2	2:J:429:GLY:H	1.65	0.60
1:M:274:ILE:HG23	1:M:306:ASN:ND2	2.09	0.60
4:P:817:MRG:H2'	4:P:818:DC:C6	2.37	0.60
1:E:465:LYS:O	1:E:466:VAL:HG12	2.01	0.60
1:A:98:ALA:HB1	1:A:349:LEU:HD22	1.83	0.60
1:E:53:GLU:CD	1:E:53:GLU:H	2.04	0.60
1:M:406:TRP:HD1	1:M:407:GLN:HE21	1.50	0.60
3:C:706:DT:H2'	3:C:707:DG:H8	1.67	0.60
1:I:218:ASP:HA	1:I:220:LYS:NZ	2.15	0.60
1:M:10:VAL:HG21	1:M:153:TRP:HH2	1.67	0.60
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.66	0.60
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.37	0.60
1:I:69:THR:HG22	1:I:69:THR:O	2.02	0.60
2:N:171:PHE:H	2:N:208:HIS:HE1	1.50	0.59
1:A:533:LEU:N	1:A:533:LEU:CD1	2.66	0.59
2:F:234:LEU:H	2:F:234:LEU:HD12	1.66	0.59
1:E:329:ILE:HG12	1:E:339:TYR:HB3	1.84	0.59
1:E:229:TRP:CE3	1:E:234:LEU:HD11	2.36	0.59
1:E:174:GLN:C	1:E:176:PRO:HD3	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.28	0.59
2:B:284:ARG:HG3	2:B:284:ARG:HH11	1.67	0.59
1:E:543:GLY:HA2	2:F:283:LEU:O	2.02	0.59
1:I:90:VAL:CG2	2:J:141:GLY:O	2.49	0.59
1:E:136:ASN:OD1	1:E:138:GLU:CG	2.50	0.59
3:C:726:DT:H2''	3:C:727:DG:C8	2.37	0.59
1:A:220:LYS:HD2	1:A:220:LYS:O	2.02	0.59
1:E:324:ASP:HA	1:E:385:LYS:HZ1	1.67	0.59
1:M:398:TRP:CZ2	1:M:411:ILE:HG12	2.37	0.59
1:M:28:GLU:HG3	1:M:135:ILE:O	2.02	0.59
1:M:74:LEU:HD13	3:O:705:DA:C5	2.37	0.59
1:M:109:LEU:HD12	1:M:109:LEU:N	2.18	0.59
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.68	0.59
2:N:169:GLU:HA	2:N:169:GLU:OE2	2.01	0.59
1:E:9:PRO:HA	1:E:121:ASP:OD2	2.03	0.59
1:E:102:LYS:H	1:E:102:LYS:CD	2.05	0.59
2:J:261:VAL:HG13	2:J:276:VAL:CG2	2.31	0.59
2:J:171:PHE:H	2:J:208:HIS:HE1	1.51	0.59
1:I:406:TRP:HD1	1:I:407:GLN:HE21	1.50	0.59
2:J:100:LEU:HD23	2:J:100:LEU:N	2.17	0.59
1:A:531:VAL:HG12	1:A:533:LEU:CD1	2.33	0.59
1:I:118:VAL:O	1:I:148:VAL:HG23	2.02	0.59
4:H:802:DA:H4'	4:H:803:DC:OP1	2.01	0.59
1:I:174:GLN:C	1:I:176:PRO:HD3	2.22	0.59
1:M:194:GLU:HA	1:M:194:GLU:OE1	2.02	0.59
2:F:125:ARG:HG2	2:F:146:TYR:O	2.02	0.59
3:O:706:DT:H2'	3:O:707:DG:C8	2.38	0.59
1:E:438:GLU:HG2	1:E:461:LYS:HD3	1.83	0.59
2:J:175:ASN:HD21	2:J:201:LYS:CE	2.15	0.59
1:A:174:GLN:C	1:A:176:PRO:HD3	2.22	0.59
1:I:303:LEU:HD13	1:I:303:LEU:O	2.03	0.59
1:E:293:ILE:CD1	1:E:294:PRO:HD2	2.29	0.59
1:M:148:VAL:O	1:M:150:PRO:HD3	2.03	0.59
2:F:171:PHE:H	2:F:208:HIS:HE1	1.51	0.59
2:N:100:LEU:N	2:N:100:LEU:HD23	2.17	0.59
1:A:320:ASP:O	1:A:343:GLN:NE2	2.36	0.59
1:M:438:GLU:OE2	1:M:463:ARG:NH1	2.35	0.59
2:N:4:PRO:HB2	2:N:7:THR:HG23	1.84	0.59
2:B:37:ILE:O	2:B:41:MET:HG3	2.03	0.59
1:I:438:GLU:OE2	1:I:463:ARG:NH1	2.35	0.59
2:N:175:ASN:HD21	2:N:201:LYS:CE	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:ARG:HH11	1:I:336:GLN:CG	2.15	0.59
1:E:406:TRP:HD1	1:E:407:GLN:HE21	1.49	0.59
1:M:447:ASN:CA	1:M:556:ILE:HD13	2.32	0.59
1:M:410:TRP:HZ3	2:N:401:TRP:CE2	2.21	0.59
1:A:102:LYS:CD	1:A:102:LYS:H	2.06	0.59
1:A:277:ARG:NH1	1:A:336:GLN:CG	2.66	0.59
4:L:817:MRG:H2'	4:L:818:DC:C6	2.37	0.59
1:A:283:LEU:HD12	1:A:283:LEU:H	1.66	0.59
1:E:76:ASP:OD1	3:G:705:DA:H4'	2.03	0.58
1:I:518:VAL:O	1:I:522:ILE:HG12	2.03	0.58
3:K:726:DT:H2''	3:K:727:DG:C8	2.37	0.58
2:J:337:TRP:HB2	2:J:354:TYR:HB3	1.85	0.58
1:I:438:GLU:HG2	1:I:461:LYS:HD3	1.86	0.58
1:M:103:LYS:HE3	1:M:179:VAL:CG2	2.32	0.58
2:N:337:TRP:HB2	2:N:354:TYR:HB3	1.86	0.58
2:N:376:THR:O	2:N:380:ILE:HG13	2.04	0.58
3:O:708:DG:H2'	3:O:709:DC:C6	2.37	0.58
1:E:531:VAL:HG12	1:E:532:TYR:N	2.16	0.58
1:E:221:HIS:HE1	1:E:228:LEU:CB	2.16	0.58
2:J:303:LEU:HD23	2:J:303:LEU:C	2.23	0.58
1:I:418:ASN:O	1:I:420:PRO:HD3	2.04	0.58
1:E:79:GLU:O	1:E:83:ARG:HD2	2.03	0.58
2:B:241:VAL:HG13	2:B:351:THR:H	1.67	0.58
1:I:98:ALA:HB1	1:I:349:LEU:HD22	1.85	0.58
1:A:277:ARG:HH11	1:A:336:GLN:CG	2.15	0.58
2:N:261:VAL:HG13	2:N:276:VAL:CG2	2.32	0.58
1:M:329:ILE:HG12	1:M:339:TYR:HB3	1.84	0.58
2:J:5:ILE:CG1	2:J:6:GLU:N	2.60	0.58
2:J:75:VAL:HG11	2:J:77:PHE:CE2	2.38	0.58
1:M:221:HIS:HE1	1:M:228:LEU:H	1.48	0.58
1:M:277:ARG:NH1	1:M:336:GLN:CG	2.67	0.58
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.33	0.58
1:E:324:ASP:HA	1:E:385:LYS:NZ	2.19	0.58
2:J:181:TYR:HA	9:J:450:HOH:O	2.04	0.58
1:E:469:LEU:N	1:E:469:LEU:HD12	2.18	0.58
2:F:60:VAL:CG1	2:F:75:VAL:HG22	2.29	0.58
2:N:149:LEU:HB3	2:N:156:SER:OG	2.03	0.58
1:A:27:THR:HG22	1:A:30:LYS:H	1.69	0.58
4:H:815:DG:H2''	4:H:816:DG:O5'	2.03	0.58
2:N:62:ALA:C	2:N:63:ILE:HG23	2.22	0.58
2:N:8:VAL:CG2	2:N:159:ILE:HD12	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:THR:OG1	2:F:143:ARG:HG2	2.03	0.58
1:I:8:VAL:HB	1:I:159:ILE:HD12	1.86	0.57
2:J:244:ILE:N	2:J:244:ILE:HD13	2.16	0.57
1:M:146:TYR:CD2	1:M:150:PRO:HB3	2.39	0.57
2:N:303:LEU:C	2:N:303:LEU:HD23	2.24	0.57
2:N:366:LYS:O	2:N:370:GLU:HG3	2.03	0.57
2:F:31:ILE:HD11	2:F:133:PRO:HG2	1.84	0.57
3:G:726:DT:H2"	3:G:727:DG:C8	2.39	0.57
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.39	0.57
2:J:17:ASP:OD2	2:J:20:LYS:HE3	2.04	0.57
1:E:277:ARG:HH12	1:E:336:GLN:HG3	1.68	0.57
2:B:303:LEU:HD21	2:B:307:ARG:NH2	2.19	0.57
2:J:26:LEU:HD12	2:J:31:ILE:HD13	1.87	0.57
1:I:218:ASP:HA	1:I:220:LYS:HZ2	1.69	0.57
2:B:72:ARG:HE	2:B:409:THR:HG22	1.68	0.57
2:F:64:LYS:HE2	2:F:69:THR:HG23	1.84	0.57
1:A:205:LEU:HD13	1:A:209:LEU:HD11	1.86	0.57
1:I:181:TYR:CE1	2:J:138:GLU:HG2	2.39	0.57
2:J:284:ARG:HH11	2:J:284:ARG:HG3	1.70	0.57
1:M:44:GLU:OE2	6:M:823:ZP4:N6R	2.37	0.57
1:E:118:VAL:HB	1:E:149:LEU:HD22	1.87	0.57
1:A:146:TYR:CD2	1:A:150:PRO:HB3	2.39	0.57
2:N:195:ILE:HG13	2:N:199:ARG:NH1	2.20	0.57
1:A:70:ARG:NH2	6:A:823:ZP4:PD	2.78	0.57
2:B:356:ARG:HG2	2:B:357:MET:N	2.19	0.57
2:F:217:PRO:HG3	9:F:444:HOH:O	2.04	0.57
2:F:17:ASP:OD2	2:F:20:LYS:HE3	2.04	0.57
3:K:707:DG:H2'	3:K:708:DG:H8	1.68	0.57
1:M:543:GLY:HA2	2:N:283:LEU:O	2.05	0.57
1:A:90:VAL:HG23	2:B:141:GLY:O	2.03	0.57
1:I:194:GLU:OE1	1:I:194:GLU:HA	2.04	0.57
2:F:252:TRP:HB3	2:F:257:ILE:HD11	1.87	0.57
2:F:284:ARG:HG3	2:F:284:ARG:HH11	1.69	0.57
1:A:394:GLN:NE2	1:A:416:PHE:CZ	2.72	0.57
2:N:336:GLN:NE2	2:N:353:LYS:HD3	2.20	0.57
2:J:274:ILE:HD12	2:J:274:ILE:N	2.19	0.57
2:N:252:TRP:HB3	2:N:257:ILE:HD11	1.87	0.57
2:F:248:GLU:HB2	2:F:307:ARG:NH1	2.20	0.57
2:B:336:GLN:NE2	2:B:353:LYS:HD3	2.19	0.57
1:E:281:LYS:HE2	1:E:284:ARG:NH1	2.19	0.57
2:F:203:GLU:O	2:F:207:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ARG:HD3	8:J:438:SWE:H2	1.86	0.57
2:N:183:TYR:CD2	2:N:380:ILE:HG21	2.40	0.57
1:I:382:ILE:HG23	2:J:136:ASN:OD1	2.05	0.57
2:B:252:TRP:HB3	2:B:257:ILE:HD11	1.87	0.57
2:F:161:GLN:HA	2:F:161:GLN:NE2	2.20	0.57
1:A:500:GLN:HB3	2:B:422:LEU:HD13	1.86	0.57
1:A:500:GLN:HG2	1:A:535:TRP:HE1	1.69	0.57
1:M:199:ARG:NH2	1:M:223:LYS:HB2	2.20	0.57
1:A:164:MET:HE2	1:A:187:LEU:HD21	1.85	0.57
1:I:410:TRP:CZ2	1:I:412:PRO:HA	2.39	0.57
1:I:91:GLN:CG	1:I:161:GLN:HE22	2.18	0.57
1:E:90:VAL:HG23	2:F:141:GLY:O	2.05	0.57
1:M:500:GLN:HB3	2:N:422:LEU:HD13	1.87	0.57
2:N:388:LYS:HG2	2:N:413:GLU:HB3	1.87	0.57
2:B:50:ILE:HG21	2:B:145:GLN:OE1	2.04	0.57
1:I:100:LEU:HD21	1:I:181:TYR:CZ	2.39	0.57
2:B:337:TRP:HB2	2:B:354:TYR:HB3	1.85	0.57
2:F:96:HIS:HA	2:F:181:TYR:CE1	2.40	0.57
2:J:203:GLU:O	2:J:207:GLN:HG2	2.05	0.57
2:J:234:LEU:HA	9:J:445:HOH:O	2.03	0.56
1:I:543:GLY:HA2	2:J:283:LEU:O	2.05	0.56
1:I:329:ILE:HG12	1:I:339:TYR:HB3	1.86	0.56
1:M:16:MET:CE	1:M:83:ARG:HG2	2.35	0.56
2:N:393:ILE:HD13	2:N:398:TRP:HB2	1.86	0.56
2:N:400:THR:HG22	2:N:401:TRP:CD2	2.40	0.56
3:O:723:DC:H2''	3:O:724:DT:O5'	2.04	0.56
2:J:241:VAL:HG13	2:J:351:THR:H	1.70	0.56
1:I:52:PRO:HA	1:I:143:ARG:HH22	1.70	0.56
2:N:17:ASP:OD2	2:N:20:LYS:HE3	2.06	0.56
2:F:274:ILE:HD12	2:F:274:ILE:N	2.20	0.56
1:I:32:LYS:NZ	1:I:135:ILE:HG21	2.21	0.56
1:E:406:TRP:CD2	2:F:420:PRO:HB3	2.40	0.56
2:F:171:PHE:HB2	2:F:208:HIS:CE1	2.39	0.56
2:F:248:GLU:HB2	2:F:307:ARG:HH12	1.70	0.56
2:F:194:GLU:OE1	2:F:194:GLU:HA	2.04	0.56
1:M:447:ASN:HB3	1:M:450:THR:OG1	2.04	0.56
1:I:557:ARG:NE	3:K:724:DT:OP2	2.39	0.56
2:F:153:TRP:CZ2	2:F:155:GLY:HA3	2.40	0.56
1:M:235:HIS:HB3	1:M:236:PRO:HD2	1.86	0.56
1:M:174:GLN:C	1:M:176:PRO:HD3	2.25	0.56
1:I:242:GLN:HB3	1:I:243:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:TRP:CD1	1:I:295:LEU:HD13	2.40	0.56
1:M:435:VAL:CA	2:N:290:THR:HG21	2.31	0.56
3:O:706:DT:H2'	3:O:707:DG:H8	1.70	0.56
3:C:707:DG:H2'	3:C:708:DG:C8	2.41	0.56
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.40	0.56
2:F:232:TYR:CD2	2:F:233:GLU:N	2.73	0.56
1:I:388:LYS:HE3	1:I:413:GLU:OE2	2.05	0.56
1:I:156:SER:N	1:I:157:PRO:CD	2.67	0.56
1:E:109:LEU:N	1:E:109:LEU:HD12	2.19	0.56
1:A:70:ARG:HH12	6:A:823:ZP4:H31	1.70	0.56
1:M:410:TRP:CZ2	1:M:412:PRO:HA	2.39	0.56
1:M:418:ASN:O	1:M:420:PRO:HD3	2.06	0.56
2:B:28:GLU:OE2	2:B:32:LYS:HE3	2.05	0.56
1:I:8:VAL:HG13	2:J:53:GLU:OE1	2.06	0.56
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.70	0.56
1:I:228:LEU:HD23	1:I:233:GLU:HG2	1.88	0.56
1:I:108:VAL:O	1:I:220:LYS:HB2	2.05	0.56
1:I:109:LEU:HD12	1:I:109:LEU:N	2.21	0.56
2:B:72:ARG:HH12	2:B:151:GLN:CD	2.09	0.56
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.87	0.56
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.88	0.56
2:J:252:TRP:HB3	2:J:257:ILE:HD11	1.88	0.56
2:J:314:VAL:CG2	2:J:315:HIS:N	2.67	0.56
2:J:366:LYS:O	2:J:370:GLU:HG3	2.05	0.56
1:M:13:LYS:HE3	1:M:84:THR:O	2.06	0.56
1:A:303:LEU:O	1:A:303:LEU:HD13	2.06	0.56
1:E:221:HIS:CD2	1:E:221:HIS:N	2.69	0.56
1:E:65:LYS:HZ2	1:E:70:ARG:HH21	1.53	0.56
1:I:281:LYS:HE2	1:I:284:ARG:NH1	2.20	0.56
1:M:324:ASP:HA	1:M:385:LYS:NZ	2.21	0.56
1:I:239:TRP:O	1:I:315:HIS:HA	2.06	0.56
1:E:407:GLN:HE22	2:F:418:ASN:HA	1.70	0.56
4:H:818:DC:H2'	4:H:819:DG:H8	1.71	0.56
1:A:70:ARG:NH2	6:A:823:ZP4:O1D	2.38	0.56
1:I:325:LEU:N	1:I:325:LEU:HD12	2.21	0.56
1:A:108:VAL:O	1:A:220:LYS:HB2	2.06	0.56
1:M:7:THR:HG22	1:M:119:PRO:HB2	1.88	0.56
1:E:221:HIS:H	1:E:221:HIS:HD2	1.48	0.56
2:F:426:TRP:N	2:F:426:TRP:CD1	2.66	0.56
2:J:372:VAL:HG13	2:J:389:PHE:CD2	2.40	0.56
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:393:ILE:HD13	2:F:398:TRP:HB2	1.87	0.56
1:M:324:ASP:HA	1:M:385:LYS:HZ1	1.71	0.56
1:M:382:ILE:O	2:N:136:ASN:HB2	2.06	0.56
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.06	0.56
1:I:255:ASN:HB2	1:I:289:LEU:HB3	1.87	0.56
2:J:6:GLU:HB2	9:J:447:HOH:O	2.06	0.55
1:M:221:HIS:H	1:M:221:HIS:CD2	2.24	0.55
2:J:426:TRP:H	2:J:426:TRP:HD1	1.48	0.55
1:M:109:LEU:HA	1:M:220:LYS:HB2	1.88	0.55
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.55
2:N:75:VAL:HG11	2:N:77:PHE:CE2	2.41	0.55
1:A:3:SER:HB3	1:A:119:PRO:HD3	1.88	0.55
3:C:705:DA:H2''	3:C:706:DT:O5'	2.06	0.55
2:N:284:ARG:HG3	2:N:284:ARG:HH11	1.71	0.55
2:B:232:TYR:CD2	2:B:233:GLU:N	2.74	0.55
1:I:49:LYS:HE3	1:I:142:ILE:HG23	1.88	0.55
2:N:325:LEU:O	2:N:387:PRO:HA	2.06	0.55
2:F:372:VAL:HG13	2:F:389:PHE:CD2	2.40	0.55
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.41	0.55
2:N:339:TYR:CD2	2:N:375:ILE:HD12	2.41	0.55
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.41	0.55
2:F:336:GLN:NE2	2:F:353:LYS:HD3	2.21	0.55
1:E:222:GLN:N	1:E:224:GLU:OE1	2.40	0.55
1:A:298:GLU:CD	1:A:298:GLU:H	2.10	0.55
2:B:423:VAL:O	2:B:423:VAL:HG12	2.07	0.55
4:L:816:DG:H2'	4:L:817:MRG:H8	1.88	0.55
1:I:115:TYR:CE2	6:I:823:ZP4:H2'A	2.41	0.55
1:I:151:GLN:OE1	6:I:823:ZP4:H2'	2.07	0.55
1:E:194:GLU:HA	1:E:194:GLU:OE1	2.06	0.55
2:B:241:VAL:HG13	2:B:351:THR:N	2.21	0.55
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.87	0.55
3:O:726:DT:H2''	3:O:727:DG:C8	2.40	0.55
1:E:410:TRP:CZ2	1:E:412:PRO:HA	2.42	0.55
1:I:264:LEU:HD12	1:I:306:ASN:ND2	2.22	0.55
1:M:102:LYS:HD2	1:M:102:LYS:N	2.12	0.55
1:M:31:ILE:O	1:M:35:VAL:HG23	2.06	0.55
1:E:303:LEU:CD1	1:E:307:ARG:HD2	2.37	0.55
2:B:426:TRP:N	2:B:426:TRP:CD1	2.65	0.55
2:J:94:ILE:CD1	2:J:161:GLN:HG2	2.36	0.55
1:I:7:THR:HG22	1:I:119:PRO:HB2	1.88	0.55
2:J:377:THR:HA	2:J:380:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:277:ARG:HH11	1:M:336:GLN:HG3	1.72	0.55
2:B:194:GLU:OE1	2:B:194:GLU:HA	2.05	0.55
2:N:314:VAL:CG2	2:N:315:HIS:N	2.68	0.55
4:D:815:DG:H2''	4:D:816:DG:O5'	2.06	0.55
1:E:557:ARG:C	1:E:558:LYS:HG2	2.26	0.55
1:A:421:PRO:O	1:A:422:LEU:HD23	2.07	0.55
1:E:418:ASN:O	1:E:420:PRO:HD3	2.07	0.55
1:E:556:ILE:HD12	1:E:556:ILE:H	1.70	0.55
1:M:52:PRO:HA	1:M:143:ARG:HH22	1.71	0.55
2:J:130:PHE:CZ	2:J:144:TYR:HB2	2.42	0.55
1:A:156:SER:N	1:A:157:PRO:CD	2.70	0.55
2:N:46:LYS:O	2:N:147:ASN:N	2.38	0.55
1:E:235:HIS:HB3	1:E:236:PRO:HD2	1.87	0.55
1:E:130:PHE:CZ	1:E:144:TYR:HB2	2.42	0.55
2:N:274:ILE:HD12	2:N:274:ILE:N	2.21	0.55
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.07	0.55
2:J:400:THR:HG22	2:J:401:TRP:CD2	2.42	0.55
2:F:333:GLY:O	2:F:334:GLN:HB2	2.07	0.55
2:F:243:PRO:HB2	2:F:244:ILE:HD13	1.89	0.55
1:E:164:MET:HE2	1:E:187:LEU:HD21	1.88	0.55
2:N:62:ALA:O	2:N:63:ILE:HG22	2.07	0.55
1:I:109:LEU:HA	1:I:220:LYS:HB2	1.89	0.55
2:F:235:HIS:C	2:F:237:ASP:H	2.10	0.55
1:I:100:LEU:CD2	1:I:181:TYR:CZ	2.89	0.54
2:N:104:LYS:HA	2:N:237:ASP:OD2	2.06	0.54
2:N:108:VAL:HG22	2:N:188:TYR:CD2	2.42	0.54
1:M:77:PHE:HB2	1:M:152:GLY:O	2.07	0.54
1:E:232:TYR:N	1:E:242:GLN:HE21	2.04	0.54
1:E:441:TYR:CD1	1:E:544:GLY:CA	2.77	0.54
2:N:372:VAL:HG13	2:N:389:PHE:CD2	2.42	0.54
2:N:194:GLU:OE1	2:N:194:GLU:HA	2.07	0.54
1:A:164:MET:CE	1:A:187:LEU:HD21	2.37	0.54
1:A:418:ASN:O	1:A:420:PRO:HD3	2.08	0.54
2:J:28:GLU:OE2	2:J:32:LYS:HE3	2.06	0.54
1:I:469:LEU:CD2	1:I:480:GLN:HG3	2.37	0.54
1:I:22:LYS:HG2	1:I:23:GLN:N	2.22	0.54
1:E:394:GLN:NE2	1:E:416:PHE:CZ	2.75	0.54
2:J:50:ILE:HG21	2:J:145:GLN:OE1	2.07	0.54
2:J:356:ARG:HG2	2:J:357:MET:H	1.71	0.54
1:M:242:GLN:HB3	1:M:243:PRO:HD2	1.90	0.54
1:A:285:GLY:N	3:C:714:DG:OP1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:HG21	1:A:477:THR:HG22	1.88	0.54
1:A:22:LYS:HG2	1:A:23:GLN:H	1.71	0.54
1:M:303:LEU:HD13	1:M:303:LEU:O	2.07	0.54
2:F:257:ILE:O	2:F:261:VAL:HG23	2.07	0.54
2:N:426:TRP:H	2:N:426:TRP:HD1	1.50	0.54
1:I:26:LEU:HD12	1:I:133:PRO:HG3	1.90	0.54
1:A:495:ILE:O	1:A:533:LEU:HA	2.07	0.54
1:I:72:ARG:NH2	6:I:823:ZP4:O3A	2.41	0.54
1:A:118:VAL:O	1:A:148:VAL:HG23	2.07	0.54
2:J:325:LEU:O	2:J:387:PRO:HA	2.08	0.54
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.89	0.54
2:B:96:HIS:HA	2:B:181:TYR:CE1	2.43	0.54
1:I:473:THR:HG21	4:L:809:DC:P	2.48	0.54
1:I:225:PRO:CB	1:I:226:PRO:CD	2.71	0.54
1:E:221:HIS:HE1	1:E:228:LEU:H	1.55	0.54
2:J:94:ILE:HG21	2:J:182:GLN:O	2.07	0.54
2:F:366:LYS:O	2:F:370:GLU:HG3	2.08	0.54
1:I:118:VAL:C	1:I:148:VAL:HG23	2.28	0.54
2:J:96:HIS:CE1	2:J:381:VAL:O	2.61	0.54
2:N:203:GLU:O	2:N:207:GLN:HG2	2.08	0.54
2:F:72:ARG:HH21	2:F:409:THR:HG22	1.72	0.54
2:F:400:THR:HG22	2:F:401:TRP:CD2	2.43	0.54
1:A:23:GLN:HE22	1:A:60:VAL:H	1.48	0.54
1:A:246:LEU:HD21	1:A:264:LEU:HD11	1.89	0.54
1:A:76:ASP:OD1	3:C:705:DA:H4'	2.07	0.54
1:M:255:ASN:HD22	1:M:289:LEU:HD22	1.72	0.54
2:N:88:TRP:CE2	2:N:154:LYS:HD2	2.43	0.54
1:M:283:LEU:HD12	1:M:283:LEU:H	1.72	0.54
1:M:301:LEU:O	1:M:304:ALA:HB3	2.08	0.54
2:F:423:VAL:O	2:F:423:VAL:HG12	2.08	0.54
1:E:116:PHE:C	1:E:148:VAL:HG21	2.28	0.54
1:E:3:SER:HB2	1:E:117:SER:O	2.08	0.54
2:N:59:PRO:HG2	2:N:76:ASP:HB3	1.89	0.54
1:I:116:PHE:C	1:I:148:VAL:HG21	2.28	0.54
1:E:252:TRP:CD1	1:E:295:LEU:HD13	2.42	0.54
1:M:399:GLU:HA	1:M:402:TRP:CD1	2.42	0.54
1:E:421:PRO:O	1:E:422:LEU:HD23	2.08	0.54
1:I:229:TRP:CE2	1:I:230:MET:CG	2.90	0.54
1:A:237:ASP:C	1:A:238:LYS:HD2	2.28	0.54
3:C:726:DT:H2"	3:C:727:DG:OP2	2.07	0.54
1:E:442:VAL:HG11	1:E:485:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:CD1	1:A:307:ARG:HD2	2.39	0.53
1:I:3:SER:HB2	1:I:117:SER:O	2.08	0.53
1:A:463:ARG:NH1	1:A:463:ARG:HB2	2.23	0.53
3:C:707:DG:H2''	3:C:708:DG:H5'	1.89	0.53
2:J:325:LEU:HD21	2:J:383:TRP:CE3	2.42	0.53
2:B:328:GLU:O	2:B:339:TYR:HA	2.09	0.53
1:A:46:LYS:O	1:A:147:ASN:HB2	2.09	0.53
2:F:244:ILE:HD13	2:F:244:ILE:N	2.17	0.53
1:I:510:PRO:O	1:I:522:ILE:HD12	2.08	0.53
2:B:366:LYS:O	2:B:370:GLU:HG3	2.08	0.53
1:M:108:VAL:HA	1:M:187:LEU:O	2.09	0.53
1:A:70:ARG:HH22	6:A:823:ZP4:PD	2.31	0.53
2:N:4:PRO:HA	2:N:119:PRO:HG3	1.90	0.53
1:A:388:LYS:HE3	1:A:413:GLU:OE2	2.08	0.53
1:I:303:LEU:CD1	1:I:307:ARG:HD2	2.38	0.53
2:B:244:ILE:CD1	2:B:244:ILE:H	2.16	0.53
2:F:94:ILE:HG21	2:F:182:GLN:O	2.07	0.53
4:P:818:DC:H2''	4:P:819:DG:H5'	1.91	0.53
2:B:339:TYR:CE2	2:B:375:ILE:HD12	2.43	0.53
2:F:339:TYR:CD2	2:F:375:ILE:HD12	2.43	0.53
2:F:130:PHE:CZ	2:F:144:TYR:HB2	2.44	0.53
1:E:164:MET:CE	1:E:168:LEU:HD11	2.39	0.53
2:N:257:ILE:O	2:N:261:VAL:HG23	2.08	0.53
1:I:27:THR:HB	1:I:30:LYS:HB2	1.91	0.53
2:B:333:GLY:O	2:B:334:GLN:HB2	2.08	0.53
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.09	0.53
1:I:406:TRP:CE2	2:J:420:PRO:HB3	2.43	0.53
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.08	0.53
1:A:73:LYS:HE3	1:A:146:TYR:CZ	2.43	0.53
2:F:26:LEU:HB2	2:F:31:ILE:CD1	2.38	0.53
1:M:237:ASP:O	1:M:238:LYS:HD2	2.08	0.53
1:E:479:LEU:HB3	1:E:517:LEU:HD13	1.91	0.53
2:N:356:ARG:HG2	2:N:357:MET:H	1.72	0.53
1:M:73:LYS:HE3	1:M:146:TYR:CE1	2.44	0.53
1:E:447:ASN:HB3	1:E:450:THR:OG1	2.09	0.53
1:I:90:VAL:HG22	1:I:90:VAL:O	2.09	0.53
1:M:164:MET:CE	1:M:187:LEU:HD21	2.38	0.53
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.43	0.53
2:J:26:LEU:HB2	2:J:31:ILE:CD1	2.39	0.53
1:I:235:HIS:HB2	1:I:238:LYS:O	2.09	0.53
3:G:707:DG:H2'	3:G:708:DG:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASN:HB2	1:E:289:LEU:HB3	1.91	0.53
1:M:280:SER:O	1:M:283:LEU:HD12	2.08	0.53
1:E:300:GLU:HA	1:E:300:GLU:OE1	2.08	0.53
2:N:131:THR:OG1	2:N:143:ARG:HG2	2.08	0.53
2:N:130:PHE:CZ	2:N:144:TYR:HB2	2.43	0.53
2:B:274:ILE:HD12	2:B:274:ILE:N	2.23	0.53
2:J:113:ASP:N	2:J:151:GLN:HE21	2.07	0.53
1:I:298:GLU:CD	1:I:298:GLU:H	2.12	0.53
2:N:76:ASP:OD1	2:N:411:ILE:HD12	2.09	0.53
4:P:815:DG:H2''	4:P:816:DG:O5'	2.09	0.53
1:A:90:VAL:HG22	1:A:90:VAL:O	2.09	0.53
1:E:181:TYR:CZ	2:F:138:GLU:HG2	2.44	0.53
3:G:712:DC:H2'	3:G:713:DC:C6	2.44	0.53
1:I:469:LEU:N	1:I:469:LEU:HD12	2.24	0.53
1:E:469:LEU:CD2	1:E:480:GLN:HG3	2.38	0.53
1:A:205:LEU:CD1	1:A:209:LEU:HD11	2.39	0.53
2:J:423:VAL:HG12	2:J:423:VAL:O	2.10	0.53
2:J:194:GLU:OE1	2:J:194:GLU:HA	2.09	0.53
1:I:447:ASN:HB2	1:I:556:ILE:HD13	1.91	0.53
2:F:337:TRP:HB2	2:F:354:TYR:HB3	1.89	0.53
1:E:340:GLN:HB3	1:E:351:THR:HG22	1.90	0.53
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.90	0.53
1:E:399:GLU:HA	1:E:402:TRP:CD1	2.44	0.53
1:M:90:VAL:HG22	2:N:140:PRO:CB	2.26	0.52
1:E:174:GLN:NE2	2:J:6:GLU:OE1	2.42	0.52
2:J:276:VAL:HG22	2:J:276:VAL:O	2.08	0.52
2:B:257:ILE:O	2:B:261:VAL:HG23	2.09	0.52
1:M:3:SER:CB	1:M:117:SER:O	2.57	0.52
1:M:510:PRO:O	1:M:522:ILE:HD12	2.09	0.52
3:K:708:DG:H2'	3:K:709:DC:C6	2.44	0.52
1:I:255:ASN:HD22	1:I:289:LEU:HD22	1.74	0.52
2:N:28:GLU:OE2	2:N:32:LYS:HE3	2.08	0.52
2:F:235:HIS:O	2:F:237:ASP:N	2.42	0.52
1:E:242:GLN:HB3	1:E:243:PRO:HD2	1.91	0.52
2:N:115:TYR:OH	2:N:157:PRO:HG3	2.08	0.52
1:M:94:ILE:HD11	3:O:708:DG:N2	2.24	0.52
2:F:421:PRO:O	2:F:424:LYS:N	2.43	0.52
1:M:40:GLU:O	1:M:44:GLU:HG3	2.09	0.52
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.90	0.52
1:E:90:VAL:HG22	1:E:90:VAL:O	2.09	0.52
1:I:421:PRO:O	1:I:422:LEU:HD23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:255:ASN:HB2	1:M:289:LEU:HB3	1.90	0.52
1:M:388:LYS:HE3	1:M:413:GLU:OE2	2.09	0.52
2:N:166:LYS:HB2	9:N:438:HOH:O	2.09	0.52
1:M:361:HIS:CD2	1:M:505:ILE:HG23	2.44	0.52
1:E:215:TYR:CD2	1:E:216:THR:N	2.78	0.52
1:M:115:TYR:HB3	1:M:149:LEU:O	2.08	0.52
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.92	0.52
2:J:96:HIS:HE1	2:J:381:VAL:O	1.93	0.52
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.90	0.52
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.44	0.52
1:M:512:LYS:O	1:M:513:SER:HB2	2.10	0.52
2:J:257:ILE:O	2:J:261:VAL:HG23	2.10	0.52
3:O:707:DG:H2'	3:O:708:DG:C8	2.45	0.52
2:N:423:VAL:HG12	2:N:423:VAL:O	2.10	0.52
1:M:8:VAL:HB	1:M:159:ILE:HD12	1.91	0.52
1:E:146:TYR:CD2	1:E:150:PRO:HB3	2.45	0.52
1:A:531:VAL:HG12	1:A:532:TYR:N	2.24	0.52
2:B:26:LEU:HD12	2:B:31:ILE:HD13	1.90	0.52
1:E:53:GLU:O	1:E:55:PRO:HD3	2.10	0.52
2:N:104:LYS:HG3	2:N:237:ASP:OD2	2.09	0.52
1:E:357:MET:HG2	1:E:367:GLN:HE22	1.75	0.52
2:N:13:LYS:HZ2	2:N:86:ASP:H	1.57	0.52
1:M:558:LYS:HE3	1:M:558:LYS:HA	1.91	0.52
1:E:214:LEU:N	1:E:214:LEU:CD2	2.73	0.52
1:A:463:ARG:HG2	1:A:464:GLN:N	2.23	0.52
2:J:242:GLN:NE2	2:J:353:LYS:HE3	2.24	0.52
1:I:399:GLU:HA	1:I:402:TRP:CD1	2.44	0.52
1:I:219:GLN:N	1:I:219:GLN:CD	2.63	0.52
2:F:271:TYR:HB2	2:F:274:ILE:CD1	2.39	0.52
2:B:199:ARG:O	2:B:202:ILE:HB	2.09	0.52
1:A:500:GLN:HG2	1:A:535:TRP:NE1	2.24	0.52
1:A:116:PHE:O	1:A:148:VAL:HG21	2.10	0.52
1:A:510:PRO:O	1:A:522:ILE:HD12	2.09	0.52
2:B:377:THR:HA	2:B:380:ILE:HD12	1.91	0.52
1:I:283:LEU:HD12	1:I:283:LEU:H	1.73	0.52
1:I:410:TRP:HZ3	2:J:401:TRP:CE2	2.28	0.52
1:E:388:LYS:HE3	1:E:413:GLU:OE2	2.09	0.52
1:M:3:SER:HB2	1:M:117:SER:O	2.10	0.52
1:A:181:TYR:CE1	2:B:138:GLU:HG2	2.45	0.52
1:I:264:LEU:HD12	1:I:306:ASN:HD22	1.73	0.52
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:156:SER:N	1:M:157:PRO:CD	2.72	0.52
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.91	0.52
1:A:171:PHE:CZ	1:A:205:LEU:HD23	2.45	0.52
2:J:161:GLN:NE2	2:J:161:GLN:HA	2.24	0.52
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.40	0.52
2:F:28:GLU:OE2	2:F:32:LYS:HE3	2.09	0.52
2:B:76:ASP:OD1	2:B:78:ARG:HB2	2.09	0.52
1:M:463:ARG:HH11	1:M:463:ARG:CB	2.23	0.52
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.09	0.52
1:M:181:TYR:HE2	2:N:136:ASN:HD22	1.56	0.52
2:F:169:GLU:OE2	2:F:169:GLU:HA	2.08	0.52
2:J:131:THR:OG1	2:J:143:ARG:HG2	2.10	0.52
1:I:237:ASP:O	1:I:238:LYS:HD2	2.10	0.52
1:I:124:PHE:CE2	1:I:153:TRP:CZ2	2.98	0.52
2:F:74:LEU:HD12	2:F:74:LEU:C	2.30	0.52
1:M:253:THR:HA	1:M:292:VAL:HA	1.92	0.52
1:E:298:GLU:H	1:E:298:GLU:CD	2.14	0.52
2:J:426:TRP:N	2:J:426:TRP:CD1	2.66	0.52
1:A:542:ILE:HG23	2:B:283:LEU:HD12	1.91	0.52
2:N:31:ILE:HD11	2:N:133:PRO:HG2	1.90	0.52
1:M:38:CYS:SG	1:M:132:ILE:HG13	2.50	0.52
1:E:53:GLU:CD	1:E:53:GLU:N	2.63	0.52
1:I:384:GLY:O	2:J:28:GLU:N	2.43	0.52
2:J:374:LYS:HE2	2:J:378:GLU:HG3	1.92	0.52
1:I:293:ILE:CD1	1:I:294:PRO:HD2	2.31	0.51
2:B:74:LEU:C	2:B:74:LEU:HD12	2.30	0.51
1:I:94:ILE:HD11	3:K:708:DG:H21	1.75	0.51
2:B:372:VAL:HG13	2:B:389:PHE:CD2	2.44	0.51
1:E:115:TYR:OH	1:E:184:MET:HE3	2.10	0.51
2:B:21:VAL:CG1	2:B:59:PRO:HD3	2.40	0.51
2:J:356:ARG:HG2	2:J:357:MET:N	2.25	0.51
2:J:85:GLN:HA	2:J:88:TRP:CE2	2.45	0.51
2:N:276:VAL:O	2:N:276:VAL:HG22	2.09	0.51
1:M:458:VAL:HG22	1:M:458:VAL:O	2.10	0.51
1:M:458:VAL:CG1	1:M:548:VAL:HG22	2.38	0.51
1:M:339:TYR:CD1	1:M:375:ILE:HD11	2.46	0.51
4:L:818:DC:H2''	4:L:819:DG:H5'	1.92	0.51
2:F:6:GLU:HA	2:F:6:GLU:OE1	2.10	0.51
2:B:17:ASP:OD2	2:B:20:LYS:HE3	2.10	0.51
2:F:115:TYR:HB3	2:F:149:LEU:HB2	1.92	0.51
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLU:HB2	2:B:307:ARG:NH1	2.26	0.51
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.46	0.51
2:J:319:TYR:OH	2:J:385:LYS:HD3	2.10	0.51
1:A:293:ILE:CD1	1:A:294:PRO:HD2	2.35	0.51
1:E:109:LEU:HA	1:E:220:LYS:HB2	1.93	0.51
1:E:260:LEU:HG	1:E:264:LEU:HD23	1.91	0.51
1:M:116:PHE:CA	1:M:148:VAL:HG21	2.40	0.51
1:I:101:LYS:HE2	1:I:321:PRO:HG3	1.91	0.51
2:J:339:TYR:CD2	2:J:375:ILE:HD12	2.45	0.51
1:I:108:VAL:HA	1:I:187:LEU:O	2.10	0.51
2:B:376:THR:HB	2:B:410:TRP:CH2	2.45	0.51
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.92	0.51
1:M:136:ASN:OD1	1:M:138:GLU:HG3	2.10	0.51
2:N:73:LYS:NZ	2:N:130:PHE:CZ	2.79	0.51
2:B:244:ILE:HD13	2:B:244:ILE:N	2.18	0.51
2:J:248:GLU:HB2	2:J:307:ARG:HH12	1.76	0.51
2:B:266:TRP:CE2	2:B:423:VAL:HG21	2.45	0.51
1:E:27:THR:CG2	1:E:30:LYS:H	2.24	0.51
3:K:707:DG:H2'	3:K:708:DG:C8	2.45	0.51
2:N:30:LYS:HE2	2:N:62:ALA:O	2.10	0.51
1:A:542:ILE:HG23	2:B:283:LEU:CD1	2.40	0.51
1:A:70:ARG:C	1:A:71:TRP:CD1	2.84	0.51
2:F:328:GLU:O	2:F:339:TYR:HA	2.11	0.51
2:N:356:ARG:HG2	2:N:357:MET:N	2.25	0.51
2:N:163:SER:HA	9:N:438:HOH:O	2.10	0.51
1:I:301:LEU:O	1:I:304:ALA:HB3	2.11	0.51
2:F:344:GLU:HA	2:F:344:GLU:OE1	2.11	0.51
2:J:73:LYS:HD3	2:J:146:TYR:OH	2.11	0.51
1:M:364:ASP:N	1:M:511:ASP:OD2	2.41	0.51
1:M:242:GLN:O	1:M:243:PRO:C	2.49	0.51
1:I:394:GLN:NE2	1:I:416:PHE:CZ	2.78	0.51
1:I:320:ASP:C	1:I:322:SER:H	2.13	0.51
2:N:388:LYS:HG2	2:N:413:GLU:O	2.11	0.51
1:A:331:LYS:HE3	1:A:364:ASP:OD1	2.10	0.51
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.93	0.51
1:M:285:GLY:N	3:O:714:DG:OP1	2.39	0.51
2:N:318:TYR:O	2:N:318:TYR:CD1	2.64	0.51
2:J:13:LYS:HB2	2:J:16:MET:HG3	1.93	0.51
2:B:17:ASP:O	2:B:83:ARG:CD	2.59	0.51
1:E:278:GLN:HG3	1:E:298:GLU:CB	2.38	0.51
2:F:325:LEU:HD21	2:F:383:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:PRO:HG3	2:J:137:ASN:O	2.11	0.51
1:A:70:ARG:NH1	6:A:823:ZP4:H31	2.24	0.51
1:E:229:TRP:CE2	1:E:230:MET:HG2	2.46	0.51
1:M:463:ARG:HG2	1:M:464:GLN:N	2.25	0.51
2:J:350:LYS:HG2	2:J:351:THR:N	2.25	0.51
1:M:300:GLU:OE1	1:M:300:GLU:HA	2.10	0.51
2:B:40:GLU:O	2:B:43:LYS:N	2.43	0.51
1:I:300:GLU:OE1	1:I:300:GLU:HA	2.10	0.51
2:F:174:GLN:O	2:F:176:PRO:HD3	2.11	0.51
1:E:2:ILE:HD11	1:E:45:GLY:O	2.11	0.51
1:A:23:GLN:HE21	1:A:60:VAL:HG22	1.76	0.50
2:F:271:TYR:HB2	2:F:274:ILE:HD13	1.94	0.50
2:J:248:GLU:HB2	2:J:307:ARG:NH1	2.25	0.50
1:I:27:THR:HB	1:I:30:LYS:CB	2.42	0.50
1:I:339:TYR:CD1	1:I:375:ILE:HD11	2.46	0.50
2:J:232:TYR:CD2	2:J:233:GLU:N	2.79	0.50
2:B:26:LEU:HB2	2:B:31:ILE:CD1	2.41	0.50
2:B:350:LYS:HG2	2:B:351:THR:N	2.26	0.50
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.76	0.50
1:I:281:LYS:O	1:I:284:ARG:HB2	2.11	0.50
3:G:707:DG:H2'	3:G:708:DG:C8	2.46	0.50
2:B:428:GLN:CG	2:B:429:GLY:N	2.73	0.50
2:B:421:PRO:O	2:B:424:LYS:N	2.44	0.50
4:D:818:DC:H2''	4:D:819:DG:H5'	1.91	0.50
2:N:244:ILE:CD1	2:N:244:ILE:H	2.24	0.50
2:J:113:ASP:HA	2:J:151:GLN:NE2	2.26	0.50
1:I:148:VAL:O	1:I:150:PRO:HD3	2.11	0.50
1:A:15:GLY:CA	2:F:165:THR:HG21	2.41	0.50
2:B:76:ASP:C	2:B:78:ARG:H	2.14	0.50
3:K:717:DC:H2''	3:K:718:DA:OP2	2.11	0.50
2:F:423:VAL:HB	2:F:426:TRP:CG	2.46	0.50
1:E:114:ALA:N	6:E:823:ZP4:N3A	2.60	0.50
2:N:95:PRO:O	2:N:181:TYR:HE1	1.94	0.50
1:A:200:THR:O	1:A:203:GLU:HB2	2.12	0.50
2:J:108:VAL:HG22	2:J:188:TYR:CD2	2.47	0.50
1:M:22:LYS:HG2	1:M:23:GLN:N	2.25	0.50
2:B:75:VAL:HG11	2:B:77:PHE:CD2	2.46	0.50
1:E:164:MET:CE	1:E:187:LEU:HD21	2.40	0.50
2:J:319:TYR:OH	2:J:321:PRO:HA	2.11	0.50
3:O:717:DC:H2''	3:O:718:DA:OP2	2.12	0.50
1:I:91:GLN:CG	1:I:161:GLN:NE2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:274:ILE:HD12	2:J:274:ILE:H	1.76	0.50
1:M:221:HIS:HE1	1:M:228:LEU:HB2	1.75	0.50
1:M:206:ARG:HG3	1:M:216:THR:HG21	1.94	0.50
2:J:72:ARG:HG3	2:J:72:ARG:HH11	1.76	0.50
2:N:31:ILE:CD1	2:N:133:PRO:HG2	2.42	0.50
2:B:247:PRO:HB3	2:B:430:GLY:C	2.32	0.50
2:J:59:PRO:HG2	2:J:76:ASP:HB3	1.93	0.50
2:F:350:LYS:HG2	2:F:351:THR:N	2.26	0.50
1:M:81:ASN:OD1	1:M:153:TRP:HA	2.11	0.50
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.76	0.50
1:E:354:TYR:CE1	1:E:356:ARG:HB3	2.47	0.50
1:I:354:TYR:CE1	1:I:356:ARG:HB3	2.47	0.50
1:M:277:ARG:HH11	1:M:336:GLN:CG	2.24	0.50
4:D:816:DG:H2'	4:D:817:MRG:H8	1.92	0.50
1:E:114:ALA:N	6:E:823:ZP4:N3B	2.59	0.50
2:N:17:ASP:O	2:N:83:ARG:CD	2.60	0.50
2:J:157:PRO:HG2	2:J:184:MET:CA	2.34	0.50
1:M:260:LEU:HG	1:M:264:LEU:HD23	1.93	0.50
1:A:53:GLU:O	1:A:55:PRO:HD3	2.12	0.50
3:C:713:DC:H2'	3:C:714:DG:C8	2.47	0.50
1:A:531:VAL:HG12	1:A:533:LEU:HD12	1.94	0.50
2:J:195:ILE:HG23	9:J:448:HOH:O	2.12	0.50
2:N:21:VAL:CG1	2:N:59:PRO:HD3	2.42	0.50
2:N:26:LEU:HB2	2:N:31:ILE:CD1	2.41	0.50
1:M:463:ARG:HH11	1:M:463:ARG:HB3	1.76	0.50
2:N:161:GLN:NE2	2:N:161:GLN:HA	2.27	0.50
2:F:374:LYS:HE2	2:F:378:GLU:OE2	2.12	0.50
1:A:281:LYS:HE2	1:A:284:ARG:NH1	2.26	0.50
2:F:67:ASP:HB3	2:F:219:LYS:CB	2.42	0.50
1:M:252:TRP:CD1	1:M:295:LEU:HD13	2.47	0.50
2:N:73:LYS:HD3	2:N:146:TYR:OH	2.12	0.50
2:J:17:ASP:O	2:J:83:ARG:CD	2.60	0.50
1:E:49:LYS:CE	1:E:142:ILE:HD12	2.34	0.50
1:M:221:HIS:CE1	1:M:228:LEU:HB2	2.47	0.50
1:I:454:LYS:HB2	1:I:552:VAL:O	2.12	0.50
2:N:248:GLU:HB2	2:N:307:ARG:HH12	1.77	0.50
1:A:120:LEU:O	1:A:121:ASP:C	2.50	0.50
2:B:422:LEU:C	2:B:424:LYS:H	2.14	0.50
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.38	0.50
1:A:406:TRP:CD2	2:B:420:PRO:HB3	2.47	0.49
1:I:72:ARG:HD3	1:I:74:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:PRO:HA	1:I:121:ASP:OD2	2.12	0.49
1:M:442:VAL:HG11	1:M:485:ALA:HB2	1.94	0.49
2:B:75:VAL:CG1	2:B:77:PHE:CD2	2.95	0.49
2:N:16:MET:HA	2:N:16:MET:CE	2.41	0.49
1:A:72:ARG:HG3	1:A:151:GLN:NE2	2.24	0.49
1:A:454:LYS:HB2	1:A:552:VAL:O	2.12	0.49
1:I:31:ILE:CG2	1:I:133:PRO:HG2	2.41	0.49
2:J:76:ASP:C	2:J:78:ARG:H	2.15	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.32	0.49
1:E:223:LYS:O	1:E:223:LYS:HG3	2.12	0.49
2:B:203:GLU:O	2:B:207:GLN:HG2	2.11	0.49
1:E:103:LYS:HE3	1:E:179:VAL:CG2	2.38	0.49
2:N:118:VAL:HG13	2:N:119:PRO:HD2	1.94	0.49
2:F:72:ARG:HE	2:F:409:THR:HG22	1.77	0.49
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.49
1:E:98:ALA:HB1	1:E:349:LEU:HD22	1.93	0.49
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.42	0.49
2:F:13:LYS:HB2	2:F:16:MET:HG3	1.95	0.49
1:M:3:SER:OG	1:M:5:ILE:HG22	2.12	0.49
1:M:70:ARG:CG	1:M:71:TRP:H	2.26	0.49
2:N:248:GLU:HB2	2:N:307:ARG:NH1	2.27	0.49
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.47	0.49
1:E:447:ASN:CB	1:E:556:ILE:HG23	2.41	0.49
3:K:705:DA:H2''	3:K:706:DT:O5'	2.12	0.49
2:F:377:THR:HA	2:F:380:ILE:HD12	1.94	0.49
4:L:815:DG:H2''	4:L:816:DG:O5'	2.12	0.49
1:I:242:GLN:O	1:I:243:PRO:C	2.50	0.49
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.95	0.49
2:J:393:ILE:HD13	2:J:398:TRP:HB2	1.94	0.49
1:E:441:TYR:HD2	1:E:496:VAL:HG22	1.77	0.49
1:M:363:ASN:HA	1:M:511:ASP:CG	2.32	0.49
4:H:820:DC:H2''	4:H:821:DC:H5'	1.93	0.49
1:A:121:ASP:OD1	1:A:121:ASP:C	2.51	0.49
2:F:59:PRO:HG2	2:F:76:ASP:HB3	1.95	0.49
1:I:557:ARG:CZ	3:K:724:DT:OP2	2.60	0.49
1:A:463:ARG:HH11	1:A:463:ARG:CB	2.26	0.49
2:J:428:GLN:HG2	2:J:429:GLY:N	2.27	0.49
1:I:408:ALA:HB3	2:J:393:ILE:HB	1.93	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.95	0.49
9:I:564:HOH:O	2:J:259:LYS:HE2	2.11	0.49
1:I:237:ASP:C	1:I:238:LYS:HD2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:16:MET:HA	2:J:16:MET:CE	2.42	0.49
3:C:712:DC:H2'	3:C:713:DC:C6	2.48	0.49
1:I:65:LYS:NZ	6:I:823:ZP4:O1D	2.34	0.49
2:N:232:TYR:CD2	2:N:233:GLU:N	2.81	0.49
1:E:232:TYR:OH	1:E:269:GLN:NE2	2.43	0.49
1:M:169:GLU:HB3	1:M:170:PRO:HD3	1.93	0.49
1:E:364:ASP:N	1:E:511:ASP:OD2	2.46	0.49
1:M:503:LEU:HD22	1:M:535:TRP:HB2	1.95	0.49
1:M:221:HIS:N	1:M:221:HIS:CD2	2.80	0.49
1:I:503:LEU:HD22	1:I:535:TRP:HB2	1.95	0.49
2:J:64:LYS:CE	2:J:69:THR:HG23	2.43	0.49
2:F:422:LEU:C	2:F:424:LYS:H	2.14	0.49
1:M:244:ILE:HG23	1:M:244:ILE:O	2.12	0.49
3:G:723:DC:H2''	3:G:724:DT:C5'	2.42	0.49
2:F:374:LYS:HE2	2:F:378:GLU:HG3	1.95	0.49
1:I:495:ILE:O	1:I:533:LEU:HA	2.12	0.49
1:A:250:ASP:CG	1:A:251:SER:H	2.15	0.49
2:F:318:TYR:O	2:F:318:TYR:CD1	2.66	0.49
1:E:503:LEU:HD22	1:E:535:TRP:HB2	1.93	0.49
1:M:2:ILE:HG22	1:M:117:SER:O	2.12	0.49
1:E:283:LEU:H	1:E:283:LEU:HD12	1.77	0.49
2:N:23:GLN:HG2	2:N:133:PRO:HD3	1.95	0.49
1:A:115:TYR:CD2	6:A:823:ZP4:H2'A	2.48	0.49
1:E:305:GLU:O	1:E:309:ILE:HG13	2.13	0.49
2:F:241:VAL:HG22	2:F:350:LYS:HG3	1.95	0.49
2:N:174:GLN:O	2:N:176:PRO:HD3	2.13	0.49
2:F:10:VAL:HG21	2:F:153:TRP:HH2	1.77	0.49
1:M:10:VAL:HG11	1:M:153:TRP:HZ2	1.77	0.49
1:E:357:MET:HG2	1:E:367:GLN:NE2	2.28	0.49
1:A:476:LYS:O	1:A:479:LEU:HB2	2.13	0.49
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.48	0.49
2:N:428:GLN:HG2	2:N:429:GLY:H	1.77	0.49
2:J:235:HIS:C	2:J:237:ASP:H	2.16	0.49
2:F:47:ILE:HG22	2:F:146:TYR:HA	1.95	0.49
2:J:125:ARG:HH11	2:J:147:ASN:HB3	1.77	0.49
2:J:83:ARG:HH11	2:J:83:ARG:HG3	1.78	0.49
1:M:225:PRO:O	1:M:234:LEU:O	2.31	0.49
2:N:115:TYR:OH	2:N:184:MET:O	2.29	0.49
6:M:823:ZP4:H6	4:P:822:2DA:H2''	1.94	0.49
2:B:247:PRO:HA	2:B:431:HIS:N	2.28	0.49
1:M:394:GLN:NE2	1:M:416:PHE:CZ	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:447:ASN:OD1	1:I:450:THR:HG23	2.12	0.49
1:I:420:PRO:HA	1:I:421:PRO:C	2.33	0.49
1:A:355:ALA:O	1:A:356:ARG:C	2.50	0.49
2:J:84:THR:O	2:J:87:PHE:HB3	2.12	0.49
1:I:264:LEU:CD1	1:I:306:ASN:HD22	2.26	0.49
2:N:376:THR:HB	2:N:410:TRP:CH2	2.48	0.49
1:M:149:LEU:HD21	1:M:159:ILE:CG2	2.43	0.49
1:M:164:MET:HE2	1:M:168:LEU:HD11	1.95	0.49
1:E:65:LYS:HZ3	1:E:70:ARG:HH21	1.61	0.49
1:I:437:ALA:HB1	1:I:492:GLU:O	2.12	0.49
1:M:264:LEU:HD12	1:M:306:ASN:HD22	1.78	0.48
1:M:303:LEU:CD1	1:M:307:ARG:HD2	2.43	0.48
1:A:221:HIS:HE1	1:A:228:LEU:CB	2.18	0.48
2:F:16:MET:HA	2:F:16:MET:CE	2.42	0.48
2:B:368:LEU:O	2:B:372:VAL:HG23	2.13	0.48
2:N:328:GLU:O	2:N:339:TYR:HA	2.13	0.48
2:N:78:ARG:HD2	2:N:412:PRO:O	2.13	0.48
1:I:118:VAL:O	1:I:148:VAL:CG2	2.61	0.48
1:E:533:LEU:N	1:E:533:LEU:HD12	2.28	0.48
2:B:83:ARG:HG3	2:B:83:ARG:HH11	1.78	0.48
1:E:420:PRO:HA	1:E:421:PRO:C	2.33	0.48
2:N:157:PRO:HG2	2:N:184:MET:CA	2.35	0.48
1:A:560:LEU:HB3	2:J:102:LYS:NZ	2.29	0.48
1:E:406:TRP:CE2	2:F:420:PRO:HB3	2.48	0.48
2:B:423:VAL:HB	2:B:426:TRP:CG	2.48	0.48
1:A:113:ASP:HB3	1:A:116:PHE:HB2	1.94	0.48
2:F:325:LEU:O	2:F:387:PRO:HA	2.13	0.48
1:I:253:THR:HA	1:I:292:VAL:HA	1.94	0.48
2:B:248:GLU:HB2	2:B:307:ARG:HH12	1.78	0.48
1:M:556:ILE:HG23	1:M:557:ARG:H	1.78	0.48
1:M:7:THR:CG2	1:M:119:PRO:HB2	2.44	0.48
2:F:72:ARG:HH12	2:F:151:GLN:CD	2.16	0.48
1:E:517:LEU:O	1:E:520:GLN:HB2	2.13	0.48
1:E:355:ALA:O	1:E:356:ARG:C	2.49	0.48
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.48	0.48
1:M:340:GLN:HB3	1:M:351:THR:HG22	1.95	0.48
2:B:139:THR:OG1	2:B:140:PRO:HD2	2.13	0.48
1:M:425:LEU:HD13	1:M:509:GLN:NE2	2.28	0.48
2:F:76:ASP:C	2:F:78:ARG:H	2.16	0.48
2:N:174:GLN:C	2:N:176:PRO:HD3	2.33	0.48
1:M:332:GLN:HG3	1:M:338:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:332:GLN:HG3	1:I:338:THR:HG23	1.95	0.48
1:E:320:ASP:OD2	1:E:323:LYS:HE2	2.13	0.48
2:B:109:LEU:N	2:B:109:LEU:HD22	2.29	0.48
1:I:435:VAL:HA	2:J:290:THR:CG2	2.35	0.48
2:F:368:LEU:O	2:F:372:VAL:HG23	2.13	0.48
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.95	0.48
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.96	0.48
2:J:21:VAL:CG1	2:J:59:PRO:HD3	2.43	0.48
1:E:224:GLU:OE1	1:E:224:GLU:N	2.46	0.48
2:F:104:LYS:HG3	2:F:237:ASP:OD2	2.13	0.48
2:F:130:PHE:CE1	2:F:144:TYR:HB2	2.48	0.48
1:I:533:LEU:HD12	1:I:533:LEU:N	2.28	0.48
1:E:495:ILE:O	1:E:533:LEU:HA	2.13	0.48
2:F:108:VAL:HG22	2:F:188:TYR:CD2	2.48	0.48
2:F:396:GLU:O	2:F:397:THR:C	2.48	0.48
1:M:305:GLU:O	1:M:309:ILE:HG13	2.13	0.48
2:B:374:LYS:HE2	2:B:378:GLU:HG3	1.96	0.48
2:J:115:TYR:HB3	2:J:149:LEU:CB	2.43	0.48
1:I:239:TRP:O	1:I:316:GLY:N	2.44	0.48
1:E:264:LEU:HD12	1:E:306:ASN:ND2	2.28	0.48
2:B:195:ILE:HG23	2:B:196:GLY:N	2.28	0.48
4:P:820:DC:H2''	4:P:821:DC:H5'	1.94	0.48
1:E:447:ASN:OD1	1:E:450:THR:HG23	2.13	0.48
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.94	0.48
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.96	0.48
2:N:85:GLN:HA	2:N:88:TRP:CE2	2.48	0.48
1:M:476:LYS:O	1:M:479:LEU:HB2	2.13	0.48
1:A:357:MET:HG2	1:A:367:GLN:NE2	2.29	0.48
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.12	0.48
1:I:239:TRP:CD1	1:I:316:GLY:O	2.67	0.48
1:E:157:PRO:HG2	1:E:158:ALA:H	1.79	0.48
1:E:76:ASP:C	1:E:78:ARG:H	2.17	0.48
2:F:274:ILE:CD1	2:F:274:ILE:H	2.25	0.48
1:E:108:VAL:C	1:E:109:LEU:HD12	2.34	0.48
2:J:422:LEU:C	2:J:424:LYS:H	2.16	0.48
1:M:220:LYS:HD2	1:M:220:LYS:O	2.12	0.48
2:N:62:ALA:C	2:N:63:ILE:CG2	2.81	0.48
1:I:408:ALA:HA	2:J:364:ASP:OD2	2.12	0.48
1:A:222:GLN:N	1:A:224:GLU:OE1	2.46	0.48
2:F:174:GLN:C	2:F:176:PRO:HD3	2.34	0.48
1:E:225:PRO:HB2	1:E:226:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:ASP:HB3	1:I:116:PHE:HB2	1.95	0.48
2:J:174:GLN:O	2:J:176:PRO:HD3	2.14	0.48
2:F:107:THR:HG23	2:F:232:TYR:HE2	1.79	0.48
1:M:136:ASN:OD1	1:M:138:GLU:CG	2.62	0.48
1:M:270:ILE:O	1:M:272:PRO:HD3	2.14	0.48
1:E:442:VAL:HG21	1:E:482:ILE:HG12	1.96	0.48
2:F:271:TYR:CD1	2:F:271:TYR:N	2.82	0.48
2:B:271:TYR:HB2	2:B:274:ILE:HD13	1.96	0.48
2:N:426:TRP:N	2:N:426:TRP:CD1	2.68	0.48
2:J:130:PHE:CE1	2:J:144:TYR:HB2	2.48	0.48
1:M:427:TYR:CD1	1:M:427:TYR:N	2.81	0.48
1:M:407:GLN:HE22	2:N:418:ASN:HA	1.77	0.48
2:B:426:TRP:H	2:B:426:TRP:HD1	1.50	0.48
2:J:195:ILE:HG23	2:J:196:GLY:N	2.29	0.48
1:A:219:GLN:N	1:A:219:GLN:CD	2.67	0.48
1:I:115:TYR:HB3	1:I:149:LEU:O	2.14	0.48
3:G:726:DT:H2''	3:G:727:DG:OP2	2.13	0.48
1:M:325:LEU:HD12	1:M:325:LEU:N	2.29	0.48
1:I:120:LEU:O	1:I:121:ASP:C	2.52	0.48
1:E:33:ALA:O	1:E:37:ILE:HG12	2.13	0.48
1:I:305:GLU:O	1:I:309:ILE:HG13	2.14	0.48
2:J:344:GLU:OE1	2:J:344:GLU:HA	2.13	0.48
1:I:441:TYR:CE1	1:I:544:GLY:CA	2.94	0.48
1:E:363:ASN:HA	1:E:511:ASP:CG	2.35	0.48
2:J:274:ILE:H	2:J:274:ILE:CD1	2.27	0.48
1:E:237:ASP:O	1:E:238:LYS:HD2	2.14	0.48
2:N:78:ARG:HD3	2:N:411:ILE:O	2.14	0.48
1:M:96:HIS:H	2:N:136:ASN:HD21	1.61	0.48
2:F:104:LYS:HA	2:F:237:ASP:OD2	2.14	0.48
2:J:319:TYR:OH	2:J:385:LYS:CD	2.62	0.48
2:J:235:HIS:O	2:J:237:ASP:N	2.45	0.48
1:M:175:ASN:HB3	1:M:178:ILE:HG12	1.95	0.48
2:N:350:LYS:HG2	2:N:351:THR:N	2.28	0.48
3:O:705:DA:H2''	3:O:706:DT:O5'	2.12	0.47
2:J:31:ILE:CD1	2:J:133:PRO:HG2	2.44	0.47
1:I:447:ASN:CB	1:I:556:ILE:HD13	2.44	0.47
1:E:120:LEU:O	1:E:121:ASP:C	2.51	0.47
2:N:422:LEU:C	2:N:424:LYS:H	2.17	0.47
3:G:713:DC:H2'	3:G:714:DG:C8	2.49	0.47
1:M:517:LEU:HD22	1:M:521:ILE:HD11	1.96	0.47
1:E:478:GLU:CG	1:E:499:SER:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:476:LYS:O	1:I:479:LEU:HB2	2.14	0.47
1:M:363:ASN:HB2	1:M:511:ASP:OD2	2.13	0.47
1:A:531:VAL:CG1	1:A:533:LEU:HD11	2.43	0.47
1:I:3:SER:CB	1:I:117:SER:O	2.62	0.47
2:F:376:THR:HB	2:F:410:TRP:CH2	2.48	0.47
2:F:319:TYR:OH	2:F:385:LYS:CD	2.61	0.47
1:M:237:ASP:C	1:M:238:LYS:HD2	2.34	0.47
1:M:315:HIS:H	1:M:315:HIS:CD2	2.32	0.47
2:B:357:MET:HB3	2:B:360:ALA:HB3	1.96	0.47
1:A:357:MET:HG2	1:A:367:GLN:HE22	1.79	0.47
2:N:38:CYS:SG	2:N:132:ILE:HD11	2.54	0.47
2:N:374:LYS:HE2	2:N:378:GLU:HG3	1.97	0.47
1:E:22:LYS:HG2	1:E:23:GLN:H	1.78	0.47
1:A:27:THR:CG2	1:A:30:LYS:H	2.27	0.47
2:B:423:VAL:HB	2:B:426:TRP:CD1	2.49	0.47
1:M:298:GLU:H	1:M:298:GLU:CD	2.18	0.47
2:F:388:LYS:HG2	2:F:413:GLU:HB3	1.96	0.47
1:I:77:PHE:O	1:I:80:LEU:N	2.48	0.47
1:A:242:GLN:O	1:A:243:PRO:C	2.53	0.47
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.13	0.47
1:A:354:TYR:CE1	1:A:356:ARG:HB3	2.49	0.47
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.97	0.47
1:M:528:LYS:HG3	1:M:531:VAL:CG2	2.44	0.47
1:I:340:GLN:HB3	1:I:351:THR:HG22	1.96	0.47
1:E:442:VAL:HB	1:E:481:ALA:HB1	1.96	0.47
2:N:83:ARG:HH11	2:N:83:ARG:HG3	1.80	0.47
2:F:115:TYR:CZ	2:F:157:PRO:HG3	2.49	0.47
2:J:271:TYR:HB2	2:J:274:ILE:CD1	2.44	0.47
2:N:13:LYS:HB2	2:N:16:MET:HG3	1.96	0.47
2:B:194:GLU:CD	2:B:195:ILE:H	2.18	0.47
2:B:94:ILE:HG21	2:B:182:GLN:O	2.14	0.47
2:N:274:ILE:H	2:N:274:ILE:HD12	1.79	0.47
2:J:328:GLU:O	2:J:339:TYR:HA	2.14	0.47
1:A:90:VAL:CG2	2:B:141:GLY:O	2.63	0.47
2:J:174:GLN:C	2:J:176:PRO:HD3	2.35	0.47
1:I:549:ASP:O	1:I:553:SER:OG	2.31	0.47
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.47
1:M:479:LEU:HB3	1:M:517:LEU:HD13	1.96	0.47
1:A:136:ASN:OD1	1:A:138:GLU:CG	2.62	0.47
2:B:396:GLU:O	2:B:397:THR:C	2.50	0.47
2:F:244:ILE:HD11	2:F:271:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:ILE:HD12	2:B:274:ILE:H	1.79	0.47
1:I:167:ILE:O	1:I:170:PRO:HD2	2.15	0.47
2:N:13:LYS:NZ	2:N:86:ASP:H	2.11	0.47
2:J:368:LEU:O	2:J:372:VAL:HG23	2.14	0.47
2:N:195:ILE:HG23	2:N:196:GLY:N	2.30	0.47
2:B:325:LEU:O	2:B:387:PRO:HA	2.14	0.47
1:M:315:HIS:N	1:M:315:HIS:CD2	2.81	0.47
1:E:250:ASP:CG	1:E:251:SER:H	2.18	0.47
1:E:395:LYS:HD3	1:E:414:TRP:CZ2	2.49	0.47
1:M:116:PHE:CE1	1:M:146:TYR:HE2	2.32	0.47
1:E:27:THR:CG2	1:E:29:GLU:HB3	2.45	0.47
1:E:244:ILE:O	1:E:244:ILE:HG23	2.14	0.47
2:B:339:TYR:CG	2:B:375:ILE:HD12	2.49	0.47
1:A:463:ARG:HH11	1:A:463:ARG:HB2	1.79	0.47
2:J:96:HIS:HA	2:J:181:TYR:CE1	2.49	0.47
3:G:717:DC:H2''	3:G:718:DA:OP2	2.14	0.47
1:I:364:ASP:N	1:I:511:ASP:OD2	2.46	0.47
1:I:246:LEU:HD11	1:I:264:LEU:HD22	1.97	0.47
1:I:303:LEU:HD13	1:I:307:ARG:HD2	1.96	0.47
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.50	0.47
2:J:271:TYR:CD1	2:J:271:TYR:N	2.82	0.47
1:M:116:PHE:HE1	1:M:146:TYR:CE2	2.32	0.47
1:E:510:PRO:O	1:E:522:ILE:HD12	2.14	0.47
1:A:511:ASP:C	1:A:511:ASP:OD1	2.53	0.47
4:H:818:DC:H2''	4:H:819:DG:H5'	1.95	0.47
1:I:325:LEU:HD13	1:I:385:LYS:HE2	1.97	0.47
2:N:402:TRP:CZ2	2:N:403:THR:HG22	2.49	0.47
1:I:221:HIS:HD2	1:I:221:HIS:H	1.62	0.47
1:M:420:PRO:HA	1:M:421:PRO:C	2.35	0.47
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.97	0.47
1:E:242:GLN:O	1:E:243:PRO:C	2.52	0.47
1:M:232:TYR:OH	1:M:269:GLN:NE2	2.45	0.47
1:E:85:GLN:O	1:E:85:GLN:HG3	2.13	0.47
1:M:225:PRO:HB2	1:M:226:PRO:CD	2.35	0.47
2:J:208:HIS:HD2	2:J:208:HIS:O	1.98	0.47
1:M:115:TYR:CZ	6:M:823:ZP4:H2'A	2.50	0.47
1:M:290:THR:O	1:M:291:GLU:C	2.52	0.47
2:F:118:VAL:HG13	2:F:119:PRO:HD2	1.96	0.47
1:I:34:LEU:HB3	1:I:132:ILE:HD12	1.96	0.47
1:A:109:LEU:N	1:A:109:LEU:CD1	2.78	0.47
2:F:72:ARG:HG3	2:F:72:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:92:LEU:HB2	2:N:158:ALA:HB1	1.95	0.47
1:I:78:ARG:O	1:I:82:LYS:HG3	2.15	0.47
1:A:305:GLU:O	1:A:309:ILE:HG13	2.15	0.47
1:I:285:GLY:O	1:I:287:LYS:HG2	2.15	0.47
3:K:712:DC:H2'	3:K:713:DC:C6	2.50	0.47
1:M:225:PRO:CB	1:M:226:PRO:HD3	2.31	0.47
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.97	0.47
2:J:374:LYS:HE2	2:J:378:GLU:OE2	2.15	0.47
1:M:354:TYR:CE1	1:M:356:ARG:HB3	2.50	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.14	0.47
3:C:717:DC:H2''	3:C:718:DA:OP2	2.14	0.47
2:J:318:TYR:CD1	2:J:318:TYR:O	2.68	0.47
1:I:434:ILE:HD12	1:I:434:ILE:N	2.30	0.47
2:B:271:TYR:N	2:B:271:TYR:CD1	2.83	0.47
1:M:315:HIS:H	1:M:315:HIS:HD2	1.63	0.47
1:M:410:TRP:CZ3	2:N:401:TRP:CE2	3.02	0.47
1:A:255:ASN:HD22	1:A:289:LEU:HD22	1.80	0.47
2:J:104:LYS:HA	2:J:237:ASP:OD2	2.15	0.47
1:I:479:LEU:HB3	1:I:517:LEU:HD13	1.96	0.47
1:M:171:PHE:HB2	1:M:208:HIS:CD2	2.50	0.47
1:I:98:ALA:O	1:I:349:LEU:CD2	2.63	0.46
2:B:244:ILE:HG12	2:B:310:LEU:HD13	1.98	0.46
2:F:195:ILE:HG23	2:F:196:GLY:N	2.30	0.46
1:M:447:ASN:OD1	1:M:450:THR:HG23	2.14	0.46
2:J:76:ASP:OD1	2:J:78:ARG:HB2	2.16	0.46
1:E:290:THR:O	1:E:291:GLU:C	2.52	0.46
2:F:17:ASP:O	2:F:83:ARG:CD	2.63	0.46
2:J:3:SER:N	2:J:4:PRO:CD	2.71	0.46
1:M:28:GLU:HA	1:M:31:ILE:HD12	1.97	0.46
2:J:253:THR:O	2:J:257:ILE:HG12	2.15	0.46
1:A:28:GLU:HA	1:A:31:ILE:HD12	1.97	0.46
1:A:72:ARG:HD3	1:A:74:LEU:HD21	1.97	0.46
2:N:271:TYR:HB2	2:N:274:ILE:CD1	2.44	0.46
1:M:558:LYS:CE	1:M:558:LYS:HA	2.45	0.46
2:B:319:TYR:OH	2:B:385:LYS:CD	2.63	0.46
1:M:16:MET:HE1	1:M:83:ARG:HG2	1.97	0.46
2:N:28:GLU:HA	2:N:135:ILE:HD11	1.97	0.46
2:J:10:VAL:HG22	2:J:87:PHE:CZ	2.49	0.46
1:M:384:GLY:O	2:N:27:THR:HA	2.16	0.46
1:M:452:LEU:HD23	1:M:470:THR:O	2.15	0.46
1:I:480:GLN:HE21	1:I:480:GLN:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:TYR:CZ	2:J:138:GLU:HG2	2.49	0.46
2:F:21:VAL:CG1	2:F:59:PRO:HD3	2.46	0.46
1:I:448:ARG:HD3	3:K:724:DT:H5''	1.97	0.46
1:A:290:THR:O	1:A:291:GLU:C	2.53	0.46
1:M:328:GLU:HG3	1:M:390:LYS:HB2	1.98	0.46
1:M:457:TYR:C	1:M:457:TYR:CD1	2.88	0.46
1:M:480:GLN:HA	1:M:480:GLN:HE21	1.80	0.46
1:I:98:ALA:O	1:I:349:LEU:HD21	2.16	0.46
2:B:16:MET:HA	2:B:16:MET:CE	2.45	0.46
1:M:46:LYS:O	1:M:147:ASN:HB2	2.16	0.46
1:I:244:ILE:HG23	1:I:244:ILE:O	2.15	0.46
1:A:225:PRO:O	1:A:234:LEU:O	2.34	0.46
2:J:216:THR:O	2:J:217:PRO:C	2.53	0.46
2:J:118:VAL:HG13	2:J:119:PRO:HD2	1.97	0.46
1:I:103:LYS:HB3	1:I:191:SER:O	2.15	0.46
2:F:253:THR:O	2:F:257:ILE:HG12	2.15	0.46
1:E:164:MET:HG3	1:E:164:MET:O	2.14	0.46
1:I:320:ASP:O	1:I:322:SER:N	2.48	0.46
2:F:242:GLN:NE2	2:F:353:LYS:HE3	2.30	0.46
2:J:84:THR:HG21	2:J:124:PHE:CZ	2.51	0.46
1:E:285:GLY:O	1:E:287:LYS:HG2	2.15	0.46
1:M:437:ALA:HB1	1:M:492:GLU:O	2.15	0.46
1:A:23:GLN:NE2	1:A:60:VAL:HG22	2.29	0.46
1:I:439:THR:HA	1:I:494:ASN:HB2	1.98	0.46
1:I:342:TYR:HA	1:I:349:LEU:HB2	1.97	0.46
1:A:303:LEU:HD11	1:A:307:ARG:NH1	2.31	0.46
1:A:303:LEU:HD13	1:A:307:ARG:HD2	1.98	0.46
2:F:261:VAL:CG1	2:F:276:VAL:HG21	2.37	0.46
2:F:85:GLN:HA	2:F:88:TRP:CE2	2.50	0.46
2:F:76:ASP:OD1	2:F:78:ARG:HB2	2.15	0.46
1:M:16:MET:HE2	1:M:83:ARG:HG2	1.98	0.46
2:F:38:CYS:SG	2:F:132:ILE:HD11	2.55	0.46
1:E:153:TRP:O	1:E:154:LYS:C	2.54	0.46
3:K:713:DC:H2'	3:K:714:DG:C8	2.51	0.46
1:E:524:GLN:O	1:E:528:LYS:HG2	2.15	0.46
1:E:511:ASP:C	1:E:511:ASP:OD1	2.55	0.46
1:E:441:TYR:CD2	1:E:496:VAL:HG22	2.50	0.46
1:M:90:VAL:HG23	2:N:141:GLY:O	2.16	0.46
1:E:49:LYS:HG3	1:E:142:ILE:HG23	1.98	0.46
2:N:423:VAL:HB	2:N:426:TRP:CG	2.50	0.46
2:N:314:VAL:HG13	2:N:317:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:VAL:C	1:M:109:LEU:HD12	2.36	0.46
4:D:820:DC:H2"	4:D:821:DC:H5'	1.96	0.46
1:A:326:ILE:O	1:A:341:ILE:HA	2.16	0.46
3:O:726:DT:H2"	3:O:727:DG:OP2	2.15	0.46
2:N:143:ARG:HG2	2:N:143:ARG:HH11	1.81	0.46
2:F:402:TRP:CZ2	2:F:403:THR:HG22	2.51	0.46
1:M:264:LEU:HD12	1:M:306:ASN:ND2	2.31	0.46
2:F:423:VAL:HB	2:F:426:TRP:CD1	2.50	0.46
1:M:118:VAL:HB	1:M:149:LEU:HD22	1.98	0.46
1:A:479:LEU:HD22	1:A:521:ILE:CD1	2.45	0.46
1:A:222:GLN:H	1:A:224:GLU:CD	2.18	0.46
1:A:136:ASN:OD1	1:A:138:GLU:HG3	2.15	0.46
1:E:332:GLN:HA	1:E:332:GLN:OE1	2.16	0.46
1:I:290:THR:O	1:I:291:GLU:C	2.54	0.46
1:M:23:GLN:NE2	1:M:60:VAL:N	2.47	0.46
2:N:253:THR:O	2:N:257:ILE:HG12	2.16	0.46
1:E:235:HIS:O	1:E:318:TYR:HE2	1.98	0.46
2:F:303:LEU:HD23	2:F:304:ALA:N	2.31	0.46
2:J:388:LYS:HG2	2:J:413:GLU:HB3	1.96	0.46
1:E:114:ALA:HB3	6:E:823:ZP4:N3'	2.30	0.46
1:M:258:CYS:HG	4:P:817:MRG:H24	1.63	0.46
1:E:476:LYS:O	1:E:479:LEU:HB2	2.16	0.46
1:E:332:GLN:HG3	1:E:338:THR:HG23	1.98	0.46
1:I:105:SER:HB3	1:I:198:HIS:CG	2.51	0.46
1:I:337:TRP:CZ3	1:I:368:LEU:HD23	2.51	0.46
1:M:460:ASN:ND2	2:N:288:ALA:HB2	2.30	0.46
1:A:67:ASN:C	1:A:69:THR:N	2.69	0.46
1:E:331:LYS:HE3	1:E:364:ASP:OD1	2.14	0.46
2:F:13:LYS:HZ1	2:F:85:GLN:H	1.64	0.46
2:N:339:TYR:CG	2:N:375:ILE:HD12	2.51	0.46
2:F:366:LYS:O	2:F:369:THR:HB	2.16	0.46
1:I:146:TYR:CD2	1:I:150:PRO:HB3	2.51	0.46
1:M:384:GLY:O	2:N:27:THR:HG22	2.16	0.46
1:M:57:ASN:HA	1:M:129:ALA:O	2.16	0.46
2:B:318:TYR:CD1	2:B:318:TYR:O	2.69	0.46
1:I:236:PRO:HG2	1:I:237:ASP:OD1	2.15	0.45
2:J:314:VAL:HG13	2:J:317:VAL:HG13	1.98	0.45
4:H:816:DG:H2'	4:H:817:MRG:H8	1.97	0.45
1:A:325:LEU:HD13	1:A:385:LYS:HE2	1.97	0.45
2:N:169:GLU:HB2	2:N:170:PRO:HD3	1.98	0.45
2:F:203:GLU:OE2	2:F:206:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:GLN:H	1:E:224:GLU:CD	2.20	0.45
1:E:479:LEU:HA	1:E:479:LEU:HD23	1.82	0.45
2:N:396:GLU:O	2:N:397:THR:C	2.55	0.45
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.16	0.45
2:N:10:VAL:HG22	2:N:87:PHE:CZ	2.51	0.45
1:M:465:LYS:O	1:M:466:VAL:HG12	2.16	0.45
1:E:10:VAL:CG1	1:E:11:LYS:N	2.78	0.45
1:I:315:HIS:N	1:I:315:HIS:CD2	2.83	0.45
1:M:76:ASP:C	1:M:78:ARG:H	2.19	0.45
2:J:423:VAL:HB	2:J:426:TRP:CG	2.50	0.45
1:I:427:TYR:OH	1:I:510:PRO:HD2	2.15	0.45
2:F:325:LEU:O	2:F:388:LYS:N	2.43	0.45
2:B:325:LEU:HB3	2:B:387:PRO:HA	1.98	0.45
2:J:339:TYR:CE2	2:J:375:ILE:HD12	2.51	0.45
1:A:115:TYR:OH	1:A:184:MET:HE3	2.16	0.45
2:F:160:PHE:CD2	2:F:164:MET:HB2	2.51	0.45
2:N:395:LYS:O	2:N:399:GLU:HG3	2.15	0.45
1:M:120:LEU:O	1:M:121:ASP:C	2.54	0.45
2:B:395:LYS:O	2:B:399:GLU:HG3	2.16	0.45
1:M:222:GLN:N	1:M:224:GLU:OE1	2.49	0.45
2:J:73:LYS:NZ	2:J:146:TYR:OH	2.48	0.45
2:J:61:PHE:CD2	2:J:403:THR:HB	2.51	0.45
2:N:325:LEU:HD21	2:N:383:TRP:CE3	2.51	0.45
2:N:199:ARG:O	2:N:202:ILE:HB	2.16	0.45
1:E:416:PHE:CD1	1:E:417:VAL:N	2.85	0.45
1:E:250:ASP:OD2	1:E:250:ASP:N	2.50	0.45
1:E:325:LEU:N	1:E:325:LEU:HD12	2.30	0.45
1:I:478:GLU:CD	1:I:499:SER:HB2	2.36	0.45
2:J:376:THR:HB	2:J:410:TRP:CH2	2.51	0.45
1:E:264:LEU:CD1	1:E:306:ASN:HD22	2.30	0.45
2:N:423:VAL:HB	2:N:426:TRP:CD1	2.51	0.45
1:M:164:MET:HE2	1:M:187:LEU:HD21	1.99	0.45
1:E:70:ARG:HH22	6:E:823:ZP4:PD	2.40	0.45
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.52	0.45
1:I:553:SER:O	1:I:556:ILE:HG23	2.17	0.45
1:M:421:PRO:O	1:M:422:LEU:HD23	2.17	0.45
1:M:325:LEU:HD13	1:M:385:LYS:HE2	1.98	0.45
3:O:712:DC:H2'	3:O:713:DC:C6	2.51	0.45
2:F:101:LYS:HD3	2:F:382:ILE:HG23	1.98	0.45
2:F:105:SER:O	2:F:190:GLY:HA2	2.16	0.45
1:M:330:GLN:HE21	1:M:330:GLN:HB2	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:CD2	1:A:441:TYR:N	2.82	0.45
1:E:86:ASP:N	1:E:86:ASP:OD1	2.50	0.45
3:K:714:DG:H2''	3:K:715:DA:C8	2.51	0.45
2:F:125:ARG:HH11	2:F:147:ASN:HB3	1.82	0.45
1:I:153:TRP:O	1:I:154:LYS:C	2.54	0.45
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.16	0.45
1:I:169:GLU:HB3	1:I:170:PRO:HD3	1.98	0.45
2:F:115:TYR:OH	2:F:157:PRO:HG3	2.17	0.45
1:I:32:LYS:HZ2	1:I:135:ILE:HG21	1.81	0.45
1:M:228:LEU:HD22	1:M:242:GLN:NE2	2.32	0.45
2:N:368:LEU:O	2:N:372:VAL:HG23	2.16	0.45
2:J:242:GLN:OE1	2:J:353:LYS:HG3	2.16	0.45
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.31	0.45
1:E:328:GLU:HG3	1:E:390:LYS:HB2	1.99	0.45
1:A:250:ASP:N	1:A:250:ASP:OD2	2.50	0.45
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.51	0.45
1:M:337:TRP:CZ3	1:M:368:LEU:HD23	2.52	0.45
1:I:315:HIS:H	1:I:315:HIS:CD2	2.35	0.45
2:F:274:ILE:CD1	2:F:274:ILE:N	2.80	0.45
1:E:108:VAL:O	1:E:220:LYS:HB2	2.17	0.45
3:O:707:DG:H2''	3:O:708:DG:C5'	2.46	0.45
2:J:69:THR:O	2:J:69:THR:HG22	2.15	0.45
1:M:149:LEU:HD21	1:M:159:ILE:HG22	1.99	0.45
2:J:423:VAL:HB	2:J:426:TRP:CD1	2.51	0.45
1:E:118:VAL:C	1:E:148:VAL:HG23	2.37	0.45
2:N:76:ASP:C	2:N:78:ARG:H	2.20	0.45
2:J:241:VAL:HG13	2:J:351:THR:N	2.32	0.45
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.52	0.45
3:O:713:DC:H2'	3:O:714:DG:C8	2.52	0.45
1:I:355:ALA:O	1:I:356:ARG:C	2.53	0.45
1:I:11:LYS:N	1:I:85:GLN:OE1	2.49	0.45
2:F:236:PRO:HA	2:F:239:TRP:CD2	2.52	0.45
1:A:106:VAL:HG12	1:A:107:THR:N	2.32	0.45
1:E:315:HIS:N	1:E:315:HIS:CD2	2.84	0.45
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.17	0.45
1:E:480:GLN:O	1:E:481:ALA:C	2.55	0.45
1:M:480:GLN:HA	1:M:480:GLN:NE2	2.31	0.45
2:N:130:PHE:CE1	2:N:144:TYR:HB2	2.51	0.45
2:F:274:ILE:HD12	2:F:274:ILE:H	1.80	0.45
1:A:264:LEU:HD12	1:A:306:ASN:HD22	1.81	0.45
2:B:274:ILE:CD1	2:B:274:ILE:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:TRP:CD1	1:E:24:TRP:C	2.90	0.45
1:A:27:THR:HG22	1:A:29:GLU:HB3	1.98	0.45
2:J:72:ARG:HH21	2:J:409:THR:CG2	2.27	0.45
1:E:398:TRP:CH2	1:E:411:ILE:HG12	2.51	0.45
2:F:216:THR:O	2:F:217:PRO:C	2.54	0.45
1:A:442:VAL:HG21	1:A:482:ILE:HG12	1.98	0.45
2:B:235:HIS:C	2:B:237:ASP:H	2.19	0.45
2:F:109:LEU:N	2:F:109:LEU:HD22	2.32	0.45
2:F:244:ILE:HG12	2:F:310:LEU:HD13	1.99	0.45
2:J:234:LEU:N	2:J:234:LEU:CD1	2.73	0.45
1:E:264:LEU:HD12	1:E:306:ASN:HD22	1.81	0.45
1:I:2:ILE:HG22	1:I:3:SER:H	1.82	0.45
2:F:174:GLN:HG3	2:F:175:ASN:OD1	2.16	0.45
1:E:209:LEU:O	1:E:212:TRP:N	2.47	0.45
1:E:121:ASP:OD1	1:E:121:ASP:C	2.55	0.45
2:J:84:THR:HG21	2:J:124:PHE:CE1	2.51	0.45
1:E:326:ILE:O	1:E:341:ILE:HA	2.17	0.45
1:E:315:HIS:CD2	1:E:315:HIS:H	2.35	0.45
2:N:320:ASP:HA	2:N:321:PRO:HD2	1.78	0.45
1:M:357:MET:HG2	1:M:367:GLN:HE22	1.82	0.45
1:I:250:ASP:N	1:I:250:ASP:OD2	2.50	0.45
1:I:480:GLN:NE2	1:I:480:GLN:HA	2.32	0.45
2:F:75:VAL:HG11	2:F:77:PHE:CD2	2.51	0.45
1:A:264:LEU:HD12	1:A:306:ASN:ND2	2.32	0.45
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.47	0.45
1:A:103:LYS:CE	1:A:179:VAL:HG21	2.42	0.45
2:B:303:LEU:HD23	2:B:304:ALA:N	2.31	0.45
1:A:108:VAL:C	1:A:109:LEU:HD12	2.36	0.45
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.82	0.45
2:N:10:VAL:HG11	2:N:124:PHE:CE1	2.51	0.45
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.52	0.45
1:E:409:THR:O	2:F:364:ASP:HB3	2.17	0.45
2:N:234:LEU:HD12	2:N:234:LEU:H	1.81	0.45
1:M:434:ILE:HD12	1:M:434:ILE:N	2.32	0.45
1:A:457:TYR:C	1:A:457:TYR:CD1	2.90	0.45
1:A:264:LEU:CD1	1:A:306:ASN:HD22	2.30	0.45
1:E:108:VAL:HA	1:E:187:LEU:O	2.17	0.45
2:B:366:LYS:O	2:B:369:THR:HB	2.17	0.45
1:A:480:GLN:NE2	1:A:480:GLN:HA	2.32	0.45
1:I:108:VAL:C	1:I:109:LEU:HD12	2.37	0.45
1:E:531:VAL:CG1	1:E:532:TYR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.99	0.45
3:G:712:DC:H2''	3:G:713:DC:O5'	2.16	0.45
1:M:93:GLY:N	2:N:137:ASN:OD1	2.49	0.45
1:M:473:THR:HG21	4:P:809:DC:P	2.57	0.45
1:E:188:TYR:C	1:E:188:TYR:CD1	2.89	0.45
1:M:293:ILE:CD1	1:M:294:PRO:HD2	2.39	0.44
1:M:244:ILE:CD1	1:M:263:LYS:HG3	2.43	0.44
2:J:421:PRO:O	2:J:424:LYS:N	2.49	0.44
2:J:325:LEU:O	2:J:388:LYS:N	2.42	0.44
1:I:398:TRP:CH2	1:I:411:ILE:HG12	2.53	0.44
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.52	0.44
2:J:396:GLU:O	2:J:397:THR:C	2.55	0.44
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.32	0.44
1:A:81:ASN:HB3	1:A:154:LYS:CD	2.47	0.44
1:I:511:ASP:OD1	1:I:511:ASP:C	2.56	0.44
1:I:433:PRO:HD3	2:J:255:ASN:OD1	2.18	0.44
1:A:512:LYS:O	1:A:513:SER:HB2	2.17	0.44
1:E:446:ALA:O	1:E:556:ILE:HG21	2.17	0.44
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.98	0.44
1:M:355:ALA:O	1:M:356:ARG:C	2.54	0.44
2:J:189:VAL:HG21	2:J:205:LEU:HD13	1.99	0.44
1:A:478:GLU:CD	1:A:499:SER:HB2	2.38	0.44
1:I:103:LYS:CE	1:I:179:VAL:HG21	2.34	0.44
1:I:4:PRO:HD2	1:I:212:TRP:O	2.16	0.44
1:A:72:ARG:CD	1:A:74:LEU:HD21	2.48	0.44
4:P:805:DG:H1'	4:P:806:DT:H5'	1.99	0.44
1:A:24:TRP:CD1	1:A:24:TRP:C	2.91	0.44
2:N:271:TYR:CD1	2:N:271:TYR:N	2.85	0.44
4:P:816:DG:H2'	4:P:817:MRG:H8	1.99	0.44
2:N:72:ARG:HH22	2:N:151:GLN:CB	2.30	0.44
1:I:164:MET:HE2	1:I:168:LEU:HD11	1.98	0.44
1:E:90:VAL:CG2	2:F:141:GLY:O	2.65	0.44
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.17	0.44
2:B:374:LYS:HE2	2:B:378:GLU:OE2	2.17	0.44
2:F:163:SER:O	2:F:164:MET:C	2.55	0.44
2:N:234:LEU:HD12	2:N:234:LEU:N	2.32	0.44
2:N:160:PHE:CD2	2:N:164:MET:HB2	2.52	0.44
1:I:315:HIS:H	1:I:315:HIS:HD2	1.66	0.44
1:E:109:LEU:N	1:E:109:LEU:CD1	2.80	0.44
1:M:115:TYR:CG	6:M:823:ZP4:H2'A	2.52	0.44
1:A:72:ARG:HG2	1:A:74:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:274:ILE:H	2:N:274:ILE:CD1	2.30	0.44
2:F:241:VAL:HG12	2:F:351:THR:OG1	2.17	0.44
2:B:72:ARG:HE	2:B:409:THR:CG2	2.30	0.44
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.33	0.44
1:I:8:VAL:CG1	2:J:53:GLU:OE1	2.66	0.44
1:I:382:ILE:HA	2:J:136:ASN:HA	1.99	0.44
2:F:339:TYR:CE2	2:F:375:ILE:HD12	2.53	0.44
3:K:726:DT:H2''	3:K:727:DG:OP2	2.16	0.44
1:M:50:ILE:CG2	1:M:145:GLN:HB3	2.46	0.44
1:I:40:GLU:O	1:I:44:GLU:HG3	2.18	0.44
1:E:96:HIS:ND1	1:E:97:PRO:HD2	2.32	0.44
2:J:118:VAL:HG22	8:J:438:SWE:C3	2.45	0.44
2:F:157:PRO:HG2	2:F:184:MET:CA	2.38	0.44
1:I:100:LEU:O	1:I:318:TYR:HB3	2.18	0.44
1:E:27:THR:HG22	1:E:29:GLU:HB3	1.98	0.44
4:L:820:DC:H2''	4:L:821:DC:H5'	1.98	0.44
1:M:209:LEU:HB3	1:M:214:LEU:CB	2.46	0.44
1:M:447:ASN:CB	1:M:556:ILE:HD13	2.47	0.44
1:M:49:LYS:HE3	1:M:142:ILE:HG23	2.00	0.44
1:M:270:ILE:HG23	1:M:314:VAL:CG2	2.48	0.44
1:E:478:GLU:CD	1:E:499:SER:HB2	2.38	0.44
1:M:342:TYR:HA	1:M:349:LEU:HB2	1.99	0.44
1:I:442:VAL:HB	1:I:481:ALA:HB1	2.00	0.44
2:F:83:ARG:HG3	2:F:83:ARG:HH11	1.83	0.44
1:I:260:LEU:HG	1:I:264:LEU:HD23	1.99	0.44
1:E:115:TYR:CG	6:E:823:ZP4:H2'A	2.52	0.44
2:N:339:TYR:CE2	2:N:375:ILE:HD12	2.52	0.44
1:E:253:THR:HA	1:E:292:VAL:HA	1.99	0.44
2:J:203:GLU:OE2	2:J:206:ARG:HD2	2.18	0.44
1:M:325:LEU:C	1:M:326:ILE:HD12	2.37	0.44
1:E:295:LEU:HB3	1:E:300:GLU:HG2	2.00	0.44
1:M:295:LEU:HB3	1:M:300:GLU:HG2	1.99	0.44
2:B:203:GLU:OE2	2:B:206:ARG:HD2	2.18	0.44
2:J:259:LYS:O	2:J:262:GLY:N	2.51	0.44
1:A:224:GLU:N	1:A:224:GLU:OE1	2.51	0.44
1:I:374:LYS:HD3	1:I:374:LYS:O	2.17	0.44
1:A:85:GLN:O	1:A:85:GLN:HG3	2.14	0.44
2:J:125:ARG:HH11	2:J:147:ASN:CB	2.31	0.44
2:N:122:GLU:HA	2:N:125:ARG:HH21	1.83	0.44
1:E:50:ILE:HG13	1:E:143:ARG:HB3	2.00	0.44
2:F:75:VAL:CG1	2:F:77:PHE:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:GLN:HG2	1:I:161:GLN:NE2	2.33	0.44
1:E:73:LYS:CE	1:E:146:TYR:OH	2.61	0.44
1:M:4:PRO:HD2	1:M:212:TRP:C	2.37	0.44
1:E:225:PRO:O	1:E:234:LEU:O	2.36	0.44
1:M:223:LYS:HG3	1:M:223:LYS:O	2.17	0.44
1:A:480:GLN:HE21	1:A:480:GLN:HA	1.82	0.44
1:A:164:MET:HE2	1:A:168:LEU:HD11	2.00	0.44
2:J:206:ARG:O	2:J:210:LEU:CD1	2.65	0.44
1:M:96:HIS:ND1	1:M:97:PRO:HD2	2.33	0.44
1:A:254:VAL:HG12	1:A:255:ASN:N	2.32	0.44
2:N:374:LYS:HE2	2:N:378:GLU:OE2	2.17	0.44
1:M:98:ALA:HB1	1:M:349:LEU:HD22	2.00	0.44
1:E:337:TRP:CZ3	1:E:368:LEU:HD23	2.53	0.44
2:N:330:GLN:HB2	2:N:338:THR:OG1	2.18	0.44
1:M:33:ALA:O	1:M:37:ILE:HG12	2.18	0.44
2:B:253:THR:OG1	2:B:256:ASP:OD1	2.34	0.44
2:B:160:PHE:CD2	2:B:164:MET:HB2	2.53	0.44
1:I:452:LEU:HD23	1:I:470:THR:O	2.18	0.44
2:F:238:LYS:HE2	2:F:238:LYS:HB2	1.80	0.44
1:I:330:GLN:HE21	1:I:330:GLN:HB2	1.57	0.44
1:A:53:GLU:CD	1:A:53:GLU:H	2.20	0.44
2:J:271:TYR:HB2	2:J:274:ILE:HD13	1.99	0.44
1:I:232:TYR:OH	1:I:269:GLN:NE2	2.48	0.44
2:F:325:LEU:HB3	2:F:387:PRO:HA	2.00	0.44
2:B:325:LEU:O	2:B:388:LYS:N	2.45	0.44
2:B:246:LEU:O	2:B:307:ARG:NH1	2.51	0.44
1:E:115:TYR:CZ	6:E:823:ZP4:H1'	2.53	0.44
2:N:76:ASP:OD1	2:N:78:ARG:HB2	2.18	0.44
2:B:339:TYR:CE2	2:B:375:ILE:HG23	2.53	0.44
2:F:23:GLN:HG2	2:F:133:PRO:HD3	1.99	0.44
1:A:173:LYS:O	1:A:176:PRO:HD3	2.18	0.44
1:I:331:LYS:HB3	1:I:421:PRO:HG2	2.00	0.44
1:I:478:GLU:CG	1:I:499:SER:HB2	2.48	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.78	0.44
1:E:22:LYS:CG	1:E:23:GLN:N	2.79	0.43
1:E:439:THR:HA	1:E:494:ASN:HB2	1.99	0.43
1:M:70:ARG:NH2	6:M:823:ZP4:H31	2.33	0.43
1:M:454:LYS:HB2	1:M:552:VAL:O	2.18	0.43
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.18	0.43
1:E:70:ARG:NH2	6:E:823:ZP4:O1D	2.51	0.43
2:F:234:LEU:H	2:F:234:LEU:CD1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:CD1	1:A:417:VAL:N	2.86	0.43
2:F:26:LEU:HB2	2:F:31:ILE:HD11	1.99	0.43
1:I:136:ASN:O	1:I:137:ASN:CB	2.66	0.43
1:A:164:MET:HG3	1:A:164:MET:O	2.17	0.43
1:I:106:VAL:HG12	1:I:107:THR:N	2.33	0.43
1:A:434:ILE:N	1:A:434:ILE:HD12	2.33	0.43
2:J:7:THR:HG22	2:J:119:PRO:HG2	2.00	0.43
1:M:303:LEU:HD13	1:M:307:ARG:HD2	2.00	0.43
1:E:439:THR:CG2	2:F:289:LEU:HD13	2.37	0.43
2:F:252:TRP:CG	2:F:295:LEU:HD11	2.52	0.43
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.98	0.43
2:N:244:ILE:HD11	2:N:271:TYR:OH	2.18	0.43
1:M:329:ILE:O	1:M:392:PRO:HD3	2.17	0.43
2:J:330:GLN:HB2	2:J:338:THR:OG1	2.18	0.43
1:E:363:ASN:OD1	1:E:365:VAL:N	2.51	0.43
1:E:512:LYS:O	1:E:513:SER:HB2	2.18	0.43
2:N:125:ARG:HH11	2:N:147:ASN:HB3	1.81	0.43
1:I:511:ASP:C	1:I:512:LYS:CG	2.87	0.43
1:M:91:GLN:HG3	1:M:161:GLN:NE2	2.32	0.43
2:J:274:ILE:N	2:J:274:ILE:CD1	2.81	0.43
1:E:303:LEU:HD13	1:E:307:ARG:HD2	1.99	0.43
2:F:234:LEU:CD1	2:F:234:LEU:N	2.78	0.43
1:I:281:LYS:HE2	1:I:284:ARG:CZ	2.48	0.43
1:I:255:ASN:O	1:I:259:LYS:HG3	2.18	0.43
2:N:357:MET:HB3	2:N:360:ALA:HB3	2.00	0.43
2:N:57:ASN:OD1	2:N:143:ARG:NH1	2.51	0.43
1:A:138:GLU:H	1:A:138:GLU:HG3	1.52	0.43
1:A:17:ASP:CG	2:F:95:PRO:HB3	2.39	0.43
1:M:478:GLU:CD	1:M:499:SER:HB2	2.39	0.43
2:B:234:LEU:N	2:B:234:LEU:HD12	2.33	0.43
1:M:91:GLN:CG	1:M:161:GLN:NE2	2.81	0.43
1:I:135:ILE:CD1	1:I:135:ILE:H	2.20	0.43
1:A:94:ILE:HD11	3:C:708:DG:H21	1.84	0.43
2:N:72:ARG:HH21	2:N:409:THR:HG22	1.83	0.43
2:N:174:GLN:HG3	2:N:175:ASN:OD1	2.19	0.43
1:M:479:LEU:HA	1:M:479:LEU:HD23	1.76	0.43
1:A:332:GLN:OE1	1:A:332:GLN:HA	2.18	0.43
2:B:237:ASP:C	2:B:239:TRP:H	2.20	0.43
2:B:174:GLN:O	2:B:176:PRO:HD3	2.18	0.43
2:F:46:LYS:HD2	2:F:116:PHE:HB3	2.01	0.43
2:N:344:GLU:HA	2:N:344:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:374:LYS:HD3	1:M:374:LYS:O	2.18	0.43
1:M:494:ASN:OD1	1:M:532:TYR:HB3	2.19	0.43
2:J:244:ILE:HD11	2:J:271:TYR:OH	2.19	0.43
1:I:49:LYS:NZ	1:I:142:ILE:HD12	2.34	0.43
1:I:232:TYR:HE1	1:I:269:GLN:NE2	2.16	0.43
1:E:219:GLN:OE1	6:E:823:ZP4:H41	2.19	0.43
1:I:209:LEU:HB3	1:I:214:LEU:CB	2.46	0.43
1:M:398:TRP:CH2	1:M:411:ILE:HG12	2.54	0.43
1:E:79:GLU:OE2	1:E:83:ARG:NH1	2.51	0.43
1:A:479:LEU:HA	1:A:479:LEU:HD23	1.74	0.43
1:E:315:HIS:HD2	1:E:315:HIS:H	1.66	0.43
1:M:250:ASP:CG	1:M:251:SER:H	2.21	0.43
1:A:165:THR:HA	1:A:182:GLN:HE22	1.83	0.43
1:A:489:SER:OG	1:A:528:LYS:HE3	2.18	0.43
1:I:317:VAL:O	1:I:349:LEU:HD23	2.18	0.43
2:N:208:HIS:O	2:N:208:HIS:HD2	2.02	0.43
1:E:547:GLN:O	1:E:548:VAL:C	2.56	0.43
1:M:113:ASP:HB3	1:M:116:PHE:HB2	1.99	0.43
2:N:420:PRO:HB2	2:N:421:PRO:HD2	2.01	0.43
2:B:202:ILE:HA	2:B:202:ILE:HD13	1.80	0.43
1:M:230:MET:C	4:P:821:DC:H5"	2.39	0.43
2:B:314:VAL:HG13	2:B:317:VAL:HG13	2.01	0.43
1:I:448:ARG:HD3	3:K:724:DT:C5'	2.49	0.43
1:E:465:LYS:O	1:E:466:VAL:CG1	2.67	0.43
3:O:714:DG:H2"	3:O:715:DA:C8	2.53	0.43
1:M:342:TYR:OH	1:M:390:LYS:HD2	2.19	0.43
2:B:174:GLN:C	2:B:176:PRO:HD3	2.39	0.43
2:J:246:LEU:HD11	2:J:264:LEU:HD21	2.00	0.43
1:M:91:GLN:CG	1:M:161:GLN:HE22	2.28	0.43
2:F:30:LYS:O	2:F:34:LEU:HB2	2.19	0.43
3:G:703:DG:H4'	3:G:704:DC:OP2	2.18	0.43
1:I:205:LEU:O	1:I:208:HIS:HB3	2.19	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	1.99	0.43
1:I:101:LYS:HG2	1:I:321:PRO:HD3	2.00	0.43
1:A:95:PRO:HD2	1:A:230:MET:HE1	1.99	0.43
2:F:5:ILE:CG2	2:F:6:GLU:N	2.80	0.43
2:F:232:TYR:CG	2:F:233:GLU:N	2.84	0.43
1:I:79:GLU:O	1:I:83:ARG:HG3	2.19	0.43
1:I:13:LYS:HE2	1:I:86:ASP:OD1	2.19	0.43
2:J:333:GLY:O	2:J:334:GLN:HB2	2.18	0.43
1:I:270:ILE:O	1:I:272:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ASP:N	2:B:123:ASP:OD2	2.51	0.43
2:J:125:ARG:NH1	2:J:147:ASN:HB3	2.34	0.43
3:C:710:DG:H2'	3:C:711:DC:C6	2.53	0.43
2:B:388:LYS:HG2	2:B:413:GLU:HB3	2.01	0.43
1:I:164:MET:CE	1:I:187:LEU:HD21	2.48	0.43
2:N:94:ILE:HG21	2:N:182:GLN:O	2.18	0.43
2:J:395:LYS:O	2:J:399:GLU:HG3	2.18	0.43
1:I:175:ASN:HB3	1:I:178:ILE:HG12	2.00	0.43
1:E:91:GLN:HG3	1:E:161:GLN:HE22	1.84	0.43
1:M:432:GLU:CG	1:M:433:PRO:HD2	2.39	0.43
2:B:157:PRO:HG2	2:B:184:MET:CA	2.40	0.43
2:N:325:LEU:HB3	2:N:387:PRO:HA	2.00	0.43
1:I:221:HIS:N	1:I:221:HIS:CD2	2.83	0.43
1:M:181:TYR:HE2	2:N:136:ASN:ND2	2.15	0.43
1:I:7:THR:CG2	1:I:119:PRO:HB2	2.49	0.43
2:J:374:LYS:HE3	2:J:374:LYS:O	2.19	0.43
1:A:201:LYS:O	1:A:204:GLU:HB2	2.19	0.43
1:I:328:GLU:HG3	1:I:390:LYS:HB2	2.01	0.43
3:G:707:DG:H2''	3:G:708:DG:C5'	2.49	0.43
1:E:406:TRP:HE1	2:F:418:ASN:CG	2.21	0.43
1:A:502:ALA:O	1:A:503:LEU:C	2.57	0.43
1:E:118:VAL:O	1:E:148:VAL:CG2	2.67	0.43
1:A:89:GLU:HG3	3:C:708:DG:OP1	2.19	0.43
1:A:427:TYR:CD1	1:A:427:TYR:N	2.87	0.43
1:M:109:LEU:N	1:M:109:LEU:CD1	2.82	0.43
1:I:451:LYS:HD3	1:I:451:LYS:HA	1.83	0.43
4:L:816:DG:H2'	4:L:817:MRG:C8	2.48	0.43
1:A:217:PRO:HB3	6:A:823:ZP4:O41	2.19	0.43
2:N:319:TYR:OH	2:N:321:PRO:HA	2.18	0.43
1:I:21:VAL:HG13	1:I:58:THR:HA	2.00	0.43
1:A:330:GLN:HE21	1:A:330:GLN:HB2	1.50	0.43
1:E:427:TYR:N	1:E:427:TYR:CD1	2.87	0.43
1:M:90:VAL:HG22	1:M:90:VAL:O	2.19	0.42
1:E:201:LYS:O	1:E:204:GLU:HB2	2.18	0.42
2:F:276:VAL:O	2:F:276:VAL:HG22	2.19	0.42
2:J:420:PRO:HB2	2:J:421:PRO:HD2	2.01	0.42
2:B:246:LEU:HD11	2:B:264:LEU:HD21	2.00	0.42
1:E:225:PRO:HD2	1:E:226:PRO:HD3	2.00	0.42
1:I:416:PHE:CD1	1:I:417:VAL:N	2.86	0.42
1:I:417:VAL:HG22	1:I:419:THR:HG22	2.01	0.42
1:I:46:LYS:HD3	1:I:116:PHE:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:174:GLN:HG3	2:J:175:ASN:OD1	2.19	0.42
1:I:303:LEU:HD11	1:I:307:ARG:NH1	2.34	0.42
1:M:246:LEU:HD11	1:M:264:LEU:HD22	2.01	0.42
1:M:439:THR:HA	1:M:494:ASN:HB2	2.01	0.42
1:I:238:LYS:HB3	1:I:315:HIS:HB2	2.00	0.42
1:I:317:VAL:HG11	1:I:347:LYS:HB3	2.00	0.42
1:E:164:MET:HE3	1:E:168:LEU:HD21	2.01	0.42
1:A:155:GLY:O	1:A:159:ILE:CG1	2.62	0.42
3:C:712:DC:H2''	3:C:713:DC:O5'	2.18	0.42
2:J:366:LYS:O	2:J:369:THR:HB	2.20	0.42
1:A:266:TRP:CE2	4:D:820:DC:H4'	2.54	0.42
1:I:479:LEU:HD23	1:I:479:LEU:HA	1.77	0.42
2:N:374:LYS:O	2:N:374:LYS:HE3	2.19	0.42
2:F:8:VAL:HB	2:F:159:ILE:HD12	2.00	0.42
1:I:99:GLY:HA2	1:I:383:TRP:NE1	2.34	0.42
1:E:429:LEU:HD11	1:E:506:ILE:HG22	2.01	0.42
8:J:438:SWE:H3'	8:J:438:SWE:H1	1.87	0.42
1:A:454:LYS:HA	1:A:467:VAL:O	2.20	0.42
1:A:542:ILE:O	1:A:545:ASN:HB3	2.19	0.42
2:N:88:TRP:CZ2	2:N:154:LYS:HD2	2.54	0.42
1:M:357:MET:HG2	1:M:367:GLN:NE2	2.33	0.42
2:B:245:VAL:HG13	2:B:245:VAL:O	2.19	0.42
3:K:711:DC:H2'	3:K:712:DC:C6	2.55	0.42
1:M:365:VAL:HG11	1:M:401:TRP:CD1	2.55	0.42
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.54	0.42
1:A:64:LYS:HE3	1:A:71:TRP:CE2	2.54	0.42
1:M:409:THR:O	2:N:364:ASP:HB3	2.20	0.42
1:M:285:GLY:O	1:M:287:LYS:HG2	2.19	0.42
2:F:66:LYS:O	2:F:67:ASP:HB2	2.19	0.42
2:F:24:TRP:CZ3	2:F:403:THR:HG21	2.54	0.42
1:E:325:LEU:C	1:E:326:ILE:HD12	2.40	0.42
1:I:486:LEU:HB3	1:I:524:GLN:HG2	2.01	0.42
1:E:452:LEU:HD23	1:E:470:THR:O	2.20	0.42
1:A:549:ASP:O	1:A:550:LYS:C	2.58	0.42
2:B:210:LEU:HD12	2:B:210:LEU:N	2.34	0.42
2:J:70:LYS:HD3	2:J:70:LYS:HA	1.78	0.42
1:E:360:ALA:O	1:E:513:SER:HA	2.19	0.42
2:B:122:GLU:HA	2:B:125:ARG:HH21	1.85	0.42
2:B:420:PRO:HB2	2:B:421:PRO:HD2	2.01	0.42
1:E:171:PHE:CE2	1:E:205:LEU:HD23	2.54	0.42
1:E:113:ASP:HA	6:E:823:ZP4:N3B	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:199:ARG:O	2:J:202:ILE:HB	2.19	0.42
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.54	0.42
1:A:325:LEU:C	1:A:326:ILE:HD12	2.40	0.42
1:E:111:VAL:HG11	1:E:214:LEU:HD13	2.01	0.42
1:A:398:TRP:CH2	1:A:411:ILE:HG12	2.54	0.42
2:F:49:LYS:HG2	2:F:144:TYR:CE1	2.55	0.42
1:E:354:TYR:HE1	1:E:356:ARG:HB3	1.84	0.42
1:I:517:LEU:HD22	1:I:521:ILE:HD11	2.02	0.42
1:M:528:LYS:HA	1:M:528:LYS:HD3	1.58	0.42
2:F:330:GLN:HB2	2:F:338:THR:OG1	2.19	0.42
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.87	0.42
1:A:86:ASP:OD1	1:A:86:ASP:N	2.53	0.42
1:M:511:ASP:C	1:M:511:ASP:OD1	2.58	0.42
1:E:204:GLU:HG2	2:J:3:SER:O	2.19	0.42
1:M:264:LEU:CD1	1:M:306:ASN:HD22	2.33	0.42
1:A:8:VAL:HB	1:A:159:ILE:HD12	2.02	0.42
2:B:350:LYS:O	2:B:351:THR:HG23	2.19	0.42
1:M:331:LYS:HB3	1:M:421:PRO:HG2	2.02	0.42
2:N:135:ILE:C	2:N:137:ASN:N	2.73	0.42
2:J:143:ARG:HH11	2:J:143:ARG:HG2	1.85	0.42
1:M:254:VAL:HG21	1:M:287:LYS:HB3	2.01	0.42
1:M:169:GLU:O	1:M:173:LYS:HG3	2.20	0.42
2:F:246:LEU:HD11	2:F:264:LEU:HD21	2.01	0.42
2:N:189:VAL:HG21	2:N:205:LEU:HD13	2.01	0.42
1:E:489:SER:OG	1:E:528:LYS:NZ	2.49	0.42
1:E:24:TRP:CZ2	3:G:704:DC:OP1	2.72	0.42
2:F:420:PRO:HB2	2:F:421:PRO:HD2	2.01	0.42
2:N:419:THR:HA	2:N:420:PRO:HD2	1.86	0.42
2:N:420:PRO:CB	2:N:421:PRO:HD2	2.50	0.42
1:M:155:GLY:O	1:M:159:ILE:CG1	2.61	0.42
2:J:420:PRO:CB	2:J:421:PRO:HD2	2.50	0.42
2:B:419:THR:HA	2:B:420:PRO:HD2	1.90	0.42
1:M:547:GLN:O	1:M:548:VAL:C	2.57	0.42
2:F:194:GLU:CD	2:F:195:ILE:H	2.23	0.42
1:A:325:LEU:HD12	1:A:325:LEU:N	2.33	0.42
2:J:350:LYS:O	2:J:351:THR:HG23	2.19	0.42
1:I:252:TRP:CD1	1:I:295:LEU:CD1	3.03	0.42
2:B:108:VAL:HB	2:B:232:TYR:OH	2.18	0.42
1:I:354:TYR:HE1	1:I:356:ARG:HB3	1.84	0.42
1:A:58:THR:HG21	1:A:77:PHE:HD1	1.85	0.42
1:M:517:LEU:O	1:M:520:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:C	1:A:69:THR:H	2.22	0.42
1:E:549:ASP:O	1:E:550:LYS:C	2.57	0.42
2:N:259:LYS:O	2:N:262:GLY:N	2.53	0.42
1:I:18:GLY:HA3	1:I:56:TYR:CE1	2.54	0.42
1:E:365:VAL:HG11	1:E:401:TRP:CD1	2.54	0.42
1:M:480:GLN:CA	1:M:480:GLN:HE21	2.31	0.42
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.54	0.42
2:J:4:PRO:HG3	2:J:119:PRO:HB3	2.01	0.42
1:I:91:GLN:HG3	1:I:161:GLN:NE2	2.29	0.42
1:E:260:LEU:HD23	1:E:279:LEU:HD22	2.02	0.42
1:I:100:LEU:HD23	1:I:181:TYR:CZ	2.55	0.42
1:E:138:GLU:HG3	1:E:138:GLU:H	1.54	0.42
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.30	0.42
1:I:116:PHE:CE1	1:I:146:TYR:HE2	2.37	0.42
1:I:116:PHE:HE1	1:I:146:TYR:HE2	1.67	0.42
2:F:241:VAL:CG1	2:F:351:THR:OG1	2.67	0.42
2:F:206:ARG:O	2:F:210:LEU:CD1	2.68	0.42
1:M:77:PHE:HB3	1:M:80:LEU:HB3	2.02	0.42
1:A:197:GLN:O	1:A:200:THR:HB	2.19	0.42
1:A:478:GLU:CG	1:A:499:SER:HB2	2.50	0.42
1:E:26:LEU:HD12	1:E:133:PRO:HG3	2.02	0.42
1:I:531:VAL:HG12	1:I:532:TYR:N	2.35	0.42
1:I:528:LYS:HA	1:I:528:LYS:HD3	1.62	0.42
1:E:18:GLY:HA3	1:E:56:TYR:CE1	2.55	0.42
1:E:486:LEU:HB3	1:E:524:GLN:HG2	2.01	0.42
1:E:331:LYS:HB3	1:E:421:PRO:HG2	2.01	0.42
1:M:480:GLN:O	1:M:481:ALA:C	2.58	0.42
1:A:486:LEU:HB3	1:A:524:GLN:HG2	2.01	0.42
2:J:402:TRP:CZ2	2:J:403:THR:HG22	2.54	0.42
1:E:74:LEU:HD13	3:G:705:DA:C5	2.55	0.42
1:I:76:ASP:OD1	3:K:705:DA:H4'	2.19	0.42
1:E:65:LYS:O	1:E:66:LYS:C	2.58	0.42
2:J:31:ILE:HD11	2:J:133:PRO:HG2	2.01	0.42
2:J:26:LEU:HB2	2:J:31:ILE:HD11	2.01	0.42
2:N:72:ARG:HG3	2:N:72:ARG:HH11	1.84	0.42
1:I:384:GLY:O	2:J:27:THR:HA	2.20	0.42
2:F:72:ARG:HH21	2:F:409:THR:CG2	2.33	0.42
1:E:338:THR:HA	1:E:353:LYS:HA	2.02	0.42
1:A:81:ASN:HB3	1:A:154:LYS:HD2	2.02	0.42
2:F:395:LYS:O	2:F:399:GLU:HG3	2.20	0.42
1:M:106:VAL:HG12	1:M:107:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:491:LEU:HD12	1:I:491:LEU:HA	1.93	0.42
1:E:330:GLN:HB2	1:E:330:GLN:HE21	1.54	0.42
1:E:302:GLU:O	1:E:306:ASN:HB2	2.20	0.42
1:E:510:PRO:HB2	1:E:522:ILE:CD1	2.43	0.42
3:C:708:DG:H2'	3:C:709:DC:H6	1.82	0.42
1:I:229:TRP:CD1	1:I:230:MET:HG2	2.55	0.42
1:M:109:LEU:HA	1:M:220:LYS:CB	2.48	0.42
2:J:107:THR:HG23	2:J:232:TYR:CE2	2.47	0.42
2:B:31:ILE:HD12	2:B:133:PRO:HG2	2.01	0.42
2:J:169:GLU:HB2	2:J:170:PRO:HD3	2.02	0.42
1:E:301:LEU:O	1:E:305:GLU:HG3	2.20	0.42
1:A:398:TRP:O	1:A:401:TRP:HB3	2.20	0.42
2:N:54:ASN:HB3	2:N:143:ARG:HH21	1.85	0.42
1:A:21:VAL:HG13	1:A:58:THR:HA	2.01	0.42
1:M:528:LYS:HG3	1:M:531:VAL:HG21	2.02	0.42
1:M:50:ILE:HG21	1:M:145:GLN:HB3	2.01	0.42
2:N:50:ILE:HG21	2:N:145:GLN:OE1	2.19	0.42
1:M:165:THR:HA	1:M:182:GLN:HE22	1.84	0.42
2:N:333:GLY:O	2:N:334:GLN:HB2	2.20	0.42
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD22	2.02	0.41
2:F:314:VAL:HG13	2:F:317:VAL:HG13	2.02	0.41
2:J:135:ILE:C	2:J:137:ASN:N	2.73	0.41
1:A:329:ILE:HD11	1:A:375:ILE:CD1	2.48	0.41
1:I:557:ARG:NH2	3:K:724:DT:OP2	2.53	0.41
1:M:463:ARG:CB	1:M:463:ARG:NH1	2.83	0.41
1:I:398:TRP:O	1:I:401:TRP:HB3	2.20	0.41
1:M:326:ILE:O	1:M:341:ILE:HA	2.20	0.41
2:N:107:THR:HG23	2:N:232:TYR:HE2	1.85	0.41
1:E:473:THR:OG1	1:E:476:LYS:HG3	2.20	0.41
1:M:317:VAL:HG11	1:M:347:LYS:HB3	2.01	0.41
1:E:434:ILE:HD12	1:E:434:ILE:N	2.35	0.41
2:F:125:ARG:HH11	2:F:147:ASN:CB	2.33	0.41
1:A:524:GLN:O	1:A:528:LYS:HG2	2.19	0.41
1:E:157:PRO:HG3	3:G:707:DG:O4'	2.20	0.41
2:F:88:TRP:CZ2	2:F:154:LYS:HD2	2.55	0.41
1:M:73:LYS:O	1:M:74:LEU:HD23	2.19	0.41
1:A:49:LYS:CE	1:A:142:ILE:HD12	2.42	0.41
1:A:49:LYS:HG3	1:A:142:ILE:HG23	2.03	0.41
1:M:109:LEU:HD23	1:M:216:THR:HG21	2.01	0.41
2:N:271:TYR:HB2	2:N:274:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:LYS:HE3	1:I:146:TYR:OH	2.20	0.41
1:I:34:LEU:H	1:I:34:LEU:HD12	1.85	0.41
2:F:210:LEU:HD12	2:F:210:LEU:N	2.35	0.41
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.50	0.41
1:E:242:GLN:HB3	1:E:243:PRO:CD	2.49	0.41
1:E:342:TYR:HA	1:E:349:LEU:HB2	2.01	0.41
1:A:517:LEU:O	1:A:520:GLN:HB2	2.20	0.41
1:E:533:LEU:CD1	1:E:533:LEU:N	2.84	0.41
1:A:338:THR:HA	1:A:353:LYS:HA	2.03	0.41
1:I:13:LYS:HA	1:I:14:PRO:HD3	1.93	0.41
1:M:281:LYS:HE2	1:M:284:ARG:NH1	2.35	0.41
1:I:172:LYS:HE2	1:I:180:ILE:HB	2.02	0.41
1:M:197:GLN:O	1:M:200:THR:HB	2.21	0.41
1:M:100:LEU:O	1:M:318:TYR:HB3	2.19	0.41
1:I:480:GLN:HE21	1:I:480:GLN:CA	2.31	0.41
1:E:528:LYS:HD3	1:E:528:LYS:HA	1.90	0.41
2:F:274:ILE:HA	2:F:306:ASN:OD1	2.19	0.41
1:M:242:GLN:HB3	1:M:243:PRO:CD	2.50	0.41
1:A:259:LYS:HA	4:D:819:DG:H5'	2.03	0.41
2:J:169:GLU:CA	2:J:169:GLU:OE2	2.66	0.41
2:F:339:TYR:CE2	2:F:375:ILE:HG23	2.55	0.41
1:E:254:VAL:HB	1:E:288:ALA:O	2.20	0.41
1:I:69:THR:CG2	1:I:69:THR:O	2.67	0.41
2:N:235:HIS:C	2:N:237:ASP:H	2.23	0.41
2:J:160:PHE:CD2	2:J:164:MET:HB2	2.55	0.41
2:B:64:LYS:CE	2:B:69:THR:CG2	2.94	0.41
1:I:178:ILE:HD12	1:I:191:SER:HB3	2.02	0.41
2:F:270:ILE:HB	2:F:271:TYR:CD1	2.55	0.41
1:A:221:HIS:N	1:A:221:HIS:HD2	2.09	0.41
1:E:257:ILE:O	1:E:260:LEU:HB3	2.19	0.41
1:A:30:LYS:O	1:A:31:ILE:C	2.57	0.41
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.41	0.41
3:K:707:DG:H2"	3:K:708:DG:C5'	2.48	0.41
2:N:26:LEU:HB2	2:N:31:ILE:HD11	2.02	0.41
1:I:63:ILE:HG21	1:I:74:LEU:HD11	2.02	0.41
2:F:135:ILE:C	2:F:137:ASN:N	2.73	0.41
2:J:242:GLN:O	2:J:242:GLN:NE2	2.54	0.41
1:I:363:ASN:OD1	1:I:365:VAL:N	2.54	0.41
2:N:94:ILE:HD11	2:N:161:GLN:HG2	2.01	0.41
1:A:97:PRO:O	1:A:100:LEU:HB2	2.20	0.41
2:B:163:SER:O	2:B:164:MET:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:146:TYR:CD2	2:F:150:PRO:HB3	2.55	0.41
1:I:153:TRP:O	1:I:155:GLY:N	2.53	0.41
1:I:277:ARG:HH12	1:I:336:GLN:HG3	1.80	0.41
2:F:420:PRO:CB	2:F:421:PRO:HD2	2.50	0.41
1:E:30:LYS:O	1:E:31:ILE:C	2.58	0.41
1:A:531:VAL:CG1	1:A:533:LEU:CD1	2.99	0.41
1:M:199:ARG:HH22	1:M:223:LYS:HB2	1.85	0.41
2:F:374:LYS:O	2:F:374:LYS:HE3	2.20	0.41
1:E:188:TYR:O	1:E:188:TYR:HD1	2.04	0.41
1:E:13:LYS:HE3	1:E:84:THR:O	2.21	0.41
2:B:270:ILE:HB	2:B:271:TYR:CD1	2.56	0.41
2:B:244:ILE:HD11	2:B:271:TYR:OH	2.19	0.41
1:I:227:PHE:HB2	1:I:234:LEU:HB2	2.03	0.41
2:J:270:ILE:HB	2:J:271:TYR:CD1	2.55	0.41
1:A:3:SER:HB2	1:A:117:SER:O	2.21	0.41
2:N:274:ILE:HA	2:N:306:ASN:OD1	2.21	0.41
2:N:274:ILE:CD1	2:N:274:ILE:N	2.84	0.41
2:F:357:MET:HB3	2:F:360:ALA:HB3	2.03	0.41
2:N:393:ILE:HG12	2:N:394:GLN:N	2.36	0.41
1:M:416:PHE:CD1	1:M:417:VAL:N	2.88	0.41
1:M:402:TRP:HB2	1:M:409:THR:HG23	2.02	0.41
1:E:342:TYR:OH	1:E:390:LYS:HD2	2.20	0.41
1:M:332:GLN:OE1	1:M:332:GLN:HA	2.20	0.41
1:I:11:LYS:O	1:I:85:GLN:HB3	2.20	0.41
4:L:805:DG:H1'	4:L:806:DT:H5'	2.03	0.41
2:N:267:ALA:O	2:N:269:GLN:N	2.53	0.41
1:I:285:GLY:O	1:I:286:THR:C	2.58	0.41
1:E:489:SER:OG	1:E:528:LYS:HE3	2.20	0.41
1:I:100:LEU:HD21	1:I:181:TYR:CD1	2.54	0.41
1:M:115:TYR:C	1:M:117:SER:H	2.24	0.41
2:F:339:TYR:CG	2:F:375:ILE:HD12	2.56	0.41
2:N:108:VAL:HB	2:N:232:TYR:OH	2.20	0.41
1:M:338:THR:HA	1:M:353:LYS:HA	2.03	0.41
1:I:332:GLN:OE1	1:I:332:GLN:HA	2.21	0.41
1:M:517:LEU:O	1:M:521:ILE:HG13	2.21	0.41
1:E:17:ASP:CG	1:E:18:GLY:H	2.23	0.41
2:F:390:LYS:NZ	2:F:415:GLU:OE2	2.53	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
1:A:223:LYS:O	1:A:223:LYS:HG3	2.20	0.41
1:E:235:HIS:O	1:E:318:TYR:CE2	2.73	0.41
2:B:337:TRP:CZ3	2:B:368:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LYS:HZ3	1:E:70:ARG:NH2	2.18	0.41
2:J:350:LYS:HG2	2:J:351:THR:H	1.86	0.41
2:J:180:ILE:HA	2:J:188:TYR:O	2.20	0.41
1:E:40:GLU:O	1:E:44:GLU:HG3	2.20	0.41
1:A:169:GLU:HB3	1:A:170:PRO:HD3	2.01	0.41
1:I:326:ILE:O	1:I:341:ILE:HA	2.20	0.41
1:I:515:SER:O	1:I:516:GLU:C	2.58	0.41
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.02	0.41
1:E:441:TYR:CD2	1:E:496:VAL:CG2	3.03	0.41
1:E:432:GLU:CG	1:E:433:PRO:HD2	2.38	0.41
2:J:267:ALA:O	2:J:270:ILE:N	2.54	0.41
1:M:116:PHE:CE1	1:M:146:TYR:CE2	3.09	0.41
1:I:207:GLN:HE22	1:I:210:LEU:HD23	1.83	0.41
1:E:446:ALA:HA	1:E:556:ILE:HG12	2.03	0.41
2:B:258:GLN:HG2	2:B:283:LEU:HD13	2.03	0.41
2:N:366:LYS:O	2:N:369:THR:HB	2.21	0.41
2:J:339:TYR:CE2	2:J:375:ILE:HG23	2.56	0.41
1:E:234:LEU:HA	1:E:234:LEU:HD23	1.78	0.41
1:E:194:GLU:O	1:E:195:ILE:C	2.59	0.41
1:I:365:VAL:HG11	1:I:401:TRP:CD1	2.56	0.41
2:F:143:ARG:HH11	2:F:143:ARG:HG2	1.86	0.41
2:B:181:TYR:CE2	2:B:183:TYR:HB2	2.56	0.41
2:N:88:TRP:CD1	2:N:154:LYS:HB2	2.56	0.41
3:O:712:DC:H2''	3:O:713:DC:O5'	2.21	0.41
2:J:12:LEU:HD22	2:J:127:TYR:CZ	2.55	0.41
1:I:102:LYS:HE2	1:I:102:LYS:HB3	1.76	0.41
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.41
1:A:270:ILE:O	1:A:272:PRO:HD3	2.21	0.41
1:A:315:HIS:N	1:A:315:HIS:CD2	2.88	0.41
2:F:202:ILE:HD13	2:F:202:ILE:HA	1.85	0.41
1:A:303:LEU:HD11	1:A:307:ARG:HH11	1.85	0.41
2:B:274:ILE:CD1	2:B:274:ILE:N	2.84	0.41
3:C:711:DC:H2'	3:C:712:DC:C6	2.56	0.41
4:H:817:MRG:H2'	4:H:818:DC:H6	1.79	0.41
1:I:109:LEU:CD1	1:I:109:LEU:N	2.83	0.41
1:A:438:GLU:CD	1:A:463:ARG:NH1	2.74	0.41
3:G:711:DC:H2'	3:G:712:DC:C6	2.56	0.41
2:J:54:ASN:HB3	2:J:143:ARG:HH21	1.86	0.41
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.20	0.41
2:B:235:HIS:O	2:B:237:ASP:N	2.50	0.41
2:F:123:ASP:N	2:F:123:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:480:GLN:O	1:I:481:ALA:C	2.59	0.40
1:E:173:LYS:O	1:E:176:PRO:HD3	2.20	0.40
2:N:74:LEU:HD12	2:N:74:LEU:C	2.42	0.40
2:J:267:ALA:C	2:J:269:GLN:N	2.73	0.40
1:I:547:GLN:O	1:I:548:VAL:C	2.59	0.40
2:B:252:TRP:CG	2:B:295:LEU:HD11	2.55	0.40
1:A:8:VAL:O	1:A:121:ASP:HB2	2.21	0.40
1:E:259:LYS:HA	4:H:819:DG:H5'	2.03	0.40
2:N:194:GLU:CD	2:N:195:ILE:H	2.24	0.40
2:N:24:TRP:CH2	2:N:403:THR:HG21	2.55	0.40
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.40
2:J:57:ASN:OD1	2:J:143:ARG:NH1	2.53	0.40
1:I:533:LEU:N	1:I:533:LEU:CD1	2.83	0.40
1:A:67:ASN:O	1:A:69:THR:N	2.54	0.40
1:A:452:LEU:HD23	1:A:470:THR:O	2.21	0.40
1:E:72:ARG:HG3	1:E:151:GLN:HE22	1.86	0.40
2:F:349:LEU:HA	2:F:349:LEU:HD23	1.87	0.40
1:I:235:HIS:CB	1:I:236:PRO:HD2	2.40	0.40
3:G:709:DC:H2"	3:G:710:DG:H5'	2.03	0.40
2:B:244:ILE:HD11	2:B:271:TYR:CE1	2.56	0.40
1:M:78:ARG:O	1:M:82:LYS:HG3	2.20	0.40
2:J:325:LEU:HB3	2:J:387:PRO:HA	2.02	0.40
1:I:94:ILE:HA	1:I:95:PRO:HD3	1.98	0.40
1:A:219:GLN:HE21	6:A:823:ZP4:H41	1.86	0.40
1:A:70:ARG:NH1	6:A:823:ZP4:C31	2.81	0.40
1:M:557:ARG:HG2	1:M:558:LYS:N	2.36	0.40
1:I:164:MET:O	1:I:164:MET:HG3	2.21	0.40
2:N:166:LYS:HD2	9:N:438:HOH:O	2.21	0.40
1:M:200:THR:O	1:M:203:GLU:HB2	2.20	0.40
1:I:460:ASN:ND2	2:J:288:ALA:HB2	2.36	0.40
1:A:215:TYR:CD2	1:A:216:THR:N	2.89	0.40
1:E:515:SER:O	1:E:516:GLU:C	2.59	0.40
2:J:349:LEU:HA	2:J:349:LEU:HD23	1.88	0.40
1:I:457:TYR:CD1	1:I:457:TYR:C	2.94	0.40
1:I:342:TYR:OH	1:I:390:LYS:HD2	2.22	0.40
2:J:30:LYS:O	2:J:34:LEU:HB2	2.21	0.40
1:I:208:HIS:O	1:I:212:TRP:HD1	2.04	0.40
1:A:547:GLN:O	1:A:548:VAL:C	2.60	0.40
2:N:78:ARG:NH1	2:N:411:ILE:HG22	2.37	0.40
2:J:339:TYR:CG	2:J:375:ILE:HD12	2.56	0.40
1:E:339:TYR:CG	1:E:375:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:CYS:SG	1:I:132:ILE:HG13	2.61	0.40
2:F:10:VAL:HG22	2:F:87:PHE:CZ	2.57	0.40
1:A:232:TYR:N	1:A:242:GLN:HE21	2.20	0.40
2:F:169:GLU:HB2	2:F:170:PRO:HD3	2.03	0.40
1:E:261:VAL:HG13	1:E:276:VAL:HG11	2.02	0.40
1:I:64:LYS:HE3	1:I:71:TRP:CH2	2.56	0.40
1:I:197:GLN:O	1:I:200:THR:HB	2.22	0.40
2:F:40:GLU:O	2:F:43:LYS:N	2.54	0.40
1:E:77:PHE:HB2	1:E:152:GLY:O	2.21	0.40
1:E:165:THR:HA	1:E:182:GLN:HE22	1.87	0.40
4:D:805:DG:H1'	4:D:806:DT:H5'	2.03	0.40
2:F:267:ALA:O	2:F:270:ILE:N	2.54	0.40
1:A:73:LYS:C	1:A:74:LEU:HD23	2.42	0.40
1:I:94:ILE:CD1	3:K:708:DG:H21	2.34	0.40
1:E:281:LYS:HE2	1:E:284:ARG:CZ	2.51	0.40
2:F:203:GLU:O	2:F:203:GLU:OE1	2.39	0.40
1:M:37:ILE:O	1:M:41:LEU:HG	2.21	0.40
1:A:315:HIS:H	1:A:315:HIS:CD2	2.40	0.40
2:F:265:ASN:O	2:F:268:SER:OG	2.34	0.40
1:M:549:ASP:O	1:M:550:LYS:C	2.59	0.40
2:B:259:LYS:O	2:B:262:GLY:N	2.54	0.40
2:B:363:ASN:O	2:B:364:ASP:C	2.59	0.40
1:M:395:LYS:HD3	1:M:414:TRP:CZ2	2.55	0.40
1:E:559:VAL:HG13	1:E:559:VAL:O	2.22	0.40
2:B:83:ARG:NH1	2:B:83:ARG:HG3	2.36	0.40
1:M:363:ASN:OD1	1:M:365:VAL:N	2.55	0.40
2:F:266:TRP:CE2	2:F:423:VAL:HG21	2.56	0.40
1:E:184:MET:HB3	1:E:185:ASP:H	1.58	0.40
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.40
1:A:203:GLU:O	1:A:207:GLN:HB2	2.22	0.40
1:A:363:ASN:OD1	1:A:365:VAL:N	2.55	0.40
2:F:43:LYS:C	2:F:45:GLY:H	2.25	0.40
2:N:97:PRO:C	2:N:99:GLY:H	2.24	0.40
1:M:542:ILE:O	1:M:545:ASN:HB3	2.21	0.40
2:F:89:GLU:O	2:F:89:GLU:HG2	2.22	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	558/562 (99%)	469 (84%)	81 (14%)	8 (1%)	14	57
1	E	558/562 (99%)	461 (83%)	85 (15%)	12 (2%)	8	45
1	I	558/562 (99%)	476 (85%)	69 (12%)	13 (2%)	8	44
1	M	558/562 (99%)	474 (85%)	70 (12%)	14 (2%)	7	41
2	B	421/437 (96%)	362 (86%)	53 (13%)	6 (1%)	14	57
2	F	415/437 (95%)	361 (87%)	42 (10%)	12 (3%)	6	36
2	J	415/437 (95%)	366 (88%)	43 (10%)	6 (1%)	14	57
2	N	415/437 (95%)	360 (87%)	47 (11%)	8 (2%)	10	50
All	All	3898/3996 (98%)	3329 (85%)	490 (13%)	79 (2%)	9	48

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
2	B	314	VAL
1	E	77	PHE
2	F	314	VAL
1	A	448	ARG
1	E	296	THR
1	E	448	ARG
2	F	136	ASN
2	F	193	LEU
1	I	122	GLU
1	I	296	THR
2	J	314	VAL
2	N	232	TYR
2	N	314	VAL
1	A	122	GLU
1	A	470	THR
2	B	136	ASN

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Mol	Chain	Res	Type
2	B	193	LEU
1	E	122	GLU
1	E	345	PRO
1	E	470	THR
1	E	554	ALA
2	F	284	ARG
1	I	318	TYR
1	I	345	PRO
1	I	448	ARG
2	J	193	LEU
2	J	284	ARG
1	M	77	PHE
1	M	122	GLU
1	M	296	THR
1	M	345	PRO
1	M	448	ARG
1	M	470	THR
1	M	554	ALA
2	N	193	LEU
1	A	291	GLU
2	B	236	PRO
1	E	291	GLU
1	E	297	GLU
2	F	5	ILE
2	F	217	PRO
1	I	277	ARG
1	I	412	PRO
1	I	470	THR
2	J	4	PRO
1	M	4	PRO
1	M	277	ARG
1	M	347	LYS
1	M	412	PRO
2	N	65	LYS
2	N	236	PRO
1	A	412	PRO
2	B	170	PRO
1	E	412	PRO
2	F	170	PRO
2	F	243	PRO
1	I	85	GLN
1	I	243	PRO

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Mol	Chain	Res	Type
1	I	291	GLU
1	M	291	GLU
2	N	170	PRO
2	N	284	ARG
2	F	236	PRO
2	J	170	PRO
1	M	243	PRO
2	N	420	PRO
2	F	213	GLY
2	F	420	PRO
2	J	420	PRO
1	A	170	PRO
1	A	243	PRO
1	E	170	PRO
1	E	243	PRO
1	I	321	PRO
2	B	420	PRO
2	F	4	PRO
1	I	170	PRO
1	M	170	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/502 (100%)	465 (93%)	35 (7%)	19	58
1	E	500/502 (100%)	470 (94%)	30 (6%)	24	65
1	I	500/502 (100%)	471 (94%)	29 (6%)	25	66
1	M	500/502 (100%)	475 (95%)	25 (5%)	30	71
2	B	375/397 (94%)	348 (93%)	27 (7%)	18	57
2	F	375/397 (94%)	347 (92%)	28 (8%)	17	55
2	J	375/397 (94%)	348 (93%)	27 (7%)	18	57
2	N	375/397 (94%)	345 (92%)	30 (8%)	15	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3500/3596 (97%)	3269 (93%)	231 (7%)	21 61

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	A	23	GLN
1	A	53	GLU
1	A	83	ARG
1	A	86	ASP
1	A	91	GLN
1	A	102	LYS
1	A	109	LEU
1	A	138	GLU
1	A	149	LEU
1	A	188	TYR
1	A	208	HIS
1	A	214	LEU
1	A	220	LYS
1	A	221	HIS
1	A	246	LEU
1	A	283	LEU
1	A	315	HIS
1	A	324	ASP
1	A	330	GLN
1	A	344	GLU
1	A	349	LEU
1	A	361	HIS
1	A	386	THR
1	A	441	TYR
1	A	458	VAL
1	A	466	VAL
1	A	496	VAL
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
1	A	548	VAL
1	A	552	VAL
1	A	556	ILE
1	A	557	ARG
2	B	24	TRP
2	B	34	LEU

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	74	LEU
2	B	100	LEU
2	B	101	LYS
2	B	120	LEU
2	B	123	ASP
2	B	139	THR
2	B	157	PRO
2	B	161	GLN
2	B	203	GLU
2	B	211	ARG
2	B	240	THR
2	B	242	GLN
2	B	244	ILE
2	B	266	TRP
2	B	271	TYR
2	B	284	ARG
2	B	286	THR
2	B	364	ASP
2	B	368	LEU
2	B	374	LYS
2	B	394	GLN
2	B	409	THR
2	B	413	GLU
2	B	426	TRP
1	E	23	GLN
1	E	53	GLU
1	E	83	ARG
1	E	86	ASP
1	E	91	GLN
1	E	102	LYS
1	E	109	LEU
1	E	138	GLU
1	E	149	LEU
1	E	172	LYS
1	E	188	TYR
1	E	214	LEU
1	E	220	LYS
1	E	221	HIS
1	E	263	LYS
1	E	283	LEU
1	E	315	HIS

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Mol	Chain	Res	Type
1	E	324	ASP
1	E	330	GLN
1	E	344	GLU
1	E	349	LEU
1	E	361	HIS
1	E	386	THR
1	E	466	VAL
1	E	496	VAL
1	E	509	GLN
1	E	517	LEU
1	E	548	VAL
1	E	557	ARG
1	E	558	LYS
2	F	3	SER
2	F	5	ILE
2	F	6	GLU
2	F	24	TRP
2	F	34	LEU
2	F	67	ASP
2	F	100	LEU
2	F	120	LEU
2	F	123	ASP
2	F	139	THR
2	F	157	PRO
2	F	161	GLN
2	F	203	GLU
2	F	211	ARG
2	F	240	THR
2	F	242	GLN
2	F	244	ILE
2	F	266	TRP
2	F	271	TYR
2	F	284	ARG
2	F	286	THR
2	F	289	LEU
2	F	364	ASP
2	F	368	LEU
2	F	374	LYS
2	F	394	GLN
2	F	413	GLU
2	F	426	TRP
1	I	2	ILE

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Mol	Chain	Res	Type
1	I	23	GLN
1	I	53	GLU
1	I	68	SER
1	I	86	ASP
1	I	91	GLN
1	I	102	LYS
1	I	109	LEU
1	I	134	SER
1	I	138	GLU
1	I	188	TYR
1	I	228	LEU
1	I	246	LEU
1	I	283	LEU
1	I	315	HIS
1	I	324	ASP
1	I	330	GLN
1	I	344	GLU
1	I	349	LEU
1	I	361	HIS
1	I	386	THR
1	I	466	VAL
1	I	496	VAL
1	I	509	GLN
1	I	512	LYS
1	I	517	LEU
1	I	548	VAL
1	I	552	VAL
1	I	556	ILE
2	J	6	GLU
2	J	24	TRP
2	J	34	LEU
2	J	67	ASP
2	J	100	LEU
2	J	120	LEU
2	J	139	THR
2	J	161	GLN
2	J	164	MET
2	J	203	GLU
2	J	211	ARG
2	J	234	LEU
2	J	240	THR
2	J	242	GLN

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Mol	Chain	Res	Type
2	J	244	ILE
2	J	266	TRP
2	J	271	TYR
2	J	275	LYS
2	J	284	ARG
2	J	286	THR
2	J	289	LEU
2	J	364	ASP
2	J	368	LEU
2	J	374	LYS
2	J	394	GLN
2	J	413	GLU
2	J	426	TRP
1	M	23	GLN
1	M	53	GLU
1	M	86	ASP
1	M	91	GLN
1	M	102	LYS
1	M	109	LEU
1	M	138	GLU
1	M	188	TYR
1	M	220	LYS
1	M	246	LEU
1	M	283	LEU
1	M	315	HIS
1	M	324	ASP
1	M	330	GLN
1	M	344	GLU
1	M	349	LEU
1	M	361	HIS
1	M	386	THR
1	M	458	VAL
1	M	466	VAL
1	M	496	VAL
1	M	517	LEU
1	M	548	VAL
1	M	556	ILE
1	M	558	LYS
2	N	5	ILE
2	N	6	GLU
2	N	24	TRP
2	N	34	LEU

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Mol	Chain	Res	Type
2	N	65	LYS
2	N	100	LEU
2	N	120	LEU
2	N	123	ASP
2	N	139	THR
2	N	161	GLN
2	N	164	MET
2	N	203	GLU
2	N	211	ARG
2	N	240	THR
2	N	242	GLN
2	N	244	ILE
2	N	266	TRP
2	N	271	TYR
2	N	275	LYS
2	N	284	ARG
2	N	286	THR
2	N	289	LEU
2	N	364	ASP
2	N	368	LEU
2	N	374	LYS
2	N	385	LYS
2	N	388	LYS
2	N	394	GLN
2	N	413	GLU
2	N	426	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	219	GLN
1	A	221	HIS
1	A	242	GLN
1	A	269	GLN
1	A	330	GLN
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	407	GLN
1	A	471	ASN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	547	GLN
2	B	174	GLN
2	B	175	ASN
2	B	197	GLN
2	B	208	HIS
2	B	278	GLN
2	B	315	HIS
2	B	336	GLN
2	B	394	GLN
2	B	407	GLN
1	E	23	GLN
1	E	161	GLN
1	E	174	GLN
1	E	182	GLN
1	E	197	GLN
1	E	207	GLN
1	E	208	HIS
1	E	221	HIS
1	E	242	GLN
1	E	255	ASN
1	E	269	GLN
1	E	330	GLN
1	E	340	GLN
1	E	407	GLN
1	E	471	ASN
1	E	480	GLN
1	E	487	GLN
1	E	509	GLN
1	E	519	ASN
1	E	520	GLN
1	E	547	GLN
2	F	161	GLN
2	F	174	GLN
2	F	175	ASN

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Mol	Chain	Res	Type
2	F	197	GLN
2	F	208	HIS
2	F	255	ASN
2	F	278	GLN
2	F	315	HIS
2	F	336	GLN
2	F	394	GLN
2	F	407	GLN
1	I	23	GLN
1	I	161	GLN
1	I	182	GLN
1	I	207	GLN
1	I	208	HIS
1	I	221	HIS
1	I	242	GLN
1	I	330	GLN
1	I	334	GLN
1	I	340	GLN
1	I	407	GLN
1	I	471	ASN
1	I	480	GLN
1	I	487	GLN
1	I	509	GLN
1	I	519	ASN
1	I	520	GLN
1	I	547	GLN
2	J	81	ASN
2	J	96	HIS
2	J	161	GLN
2	J	174	GLN
2	J	175	ASN
2	J	197	GLN
2	J	208	HIS
2	J	278	GLN
2	J	315	HIS
2	J	336	GLN
2	J	394	GLN
2	J	407	GLN
1	M	23	GLN
1	M	161	GLN
1	M	182	GLN
1	M	197	GLN

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Mol	Chain	Res	Type
1	M	207	GLN
1	M	221	HIS
1	M	315	HIS
1	M	330	GLN
1	M	334	GLN
1	M	340	GLN
1	M	407	GLN
1	M	471	ASN
1	M	480	GLN
1	M	487	GLN
1	M	509	GLN
1	M	519	ASN
1	M	520	GLN
1	M	547	GLN
2	N	81	ASN
2	N	96	HIS
2	N	174	GLN
2	N	175	ASN
2	N	197	GLN
2	N	208	HIS
2	N	269	GLN
2	N	278	GLN
2	N	315	HIS
2	N	336	GLN
2	N	394	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MRG	D	817	1,3,4	20,28,29	1.59	2 (10%)	25,39,42	3.68	8 (32%)
4	2DA	D	822	3,4	14,22,23	0.80	0	13,31,34	1.25	1 (7%)
4	MRG	H	817	1,3,4	20,28,29	1.70	2 (10%)	25,39,42	3.69	7 (28%)
4	2DA	H	822	3,4	14,22,23	0.56	0	13,31,34	0.95	1 (7%)
4	MRG	L	817	1,3,4	20,28,29	1.43	2 (10%)	25,39,42	3.68	7 (28%)
4	2DA	L	822	3,4	14,22,23	0.52	0	13,31,34	1.13	1 (7%)
4	MRG	P	817	3,4	20,28,29	1.56	2 (10%)	25,39,42	3.69	8 (32%)
4	2DA	P	822	3,4	14,22,23	0.54	0	13,31,34	1.07	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRG	D	817	1,3,4	-	0/8/26/27	0/3/3/3
4	2DA	D	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	H	817	1,3,4	-	0/8/26/27	0/3/3/3
4	2DA	H	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	L	817	1,3,4	-	0/8/26/27	0/3/3/3
4	2DA	L	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	P	817	3,4	-	0/8/26/27	0/3/3/3
4	2DA	P	822	3,4	-	0/3/18/19	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	817	MRG	C21-N2	-5.59	1.33	1.46
4	D	817	MRG	C21-N2	-5.08	1.34	1.46
4	P	817	MRG	C21-N2	-5.03	1.34	1.46
4	L	817	MRG	C21-N2	-4.62	1.35	1.46
4	L	817	MRG	C6-N1	3.43	1.39	1.33
4	D	817	MRG	C6-N1	3.63	1.39	1.33
4	H	817	MRG	C6-N1	3.73	1.40	1.33
4	P	817	MRG	C6-N1	3.79	1.40	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	817	MRG	C21-N2-C2	-12.63	99.92	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	817	MRG	C21-N2-C2	-12.55	100.06	123.80
4	L	817	MRG	C21-N2-C2	-12.52	100.11	123.80
4	H	817	MRG	C21-N2-C2	-12.34	100.45	123.80
4	H	817	MRG	C5-C6-N1	-9.21	111.00	123.59
4	P	817	MRG	C5-C6-N1	-8.97	111.33	123.59
4	L	817	MRG	C5-C6-N1	-8.91	111.41	123.59
4	D	817	MRG	C5-C6-N1	-8.83	111.52	123.59
4	H	817	MRG	C23-C22-C21	-4.28	99.00	113.12
4	P	817	MRG	C23-C22-C21	-4.24	99.11	113.12
4	L	817	MRG	C23-C22-C21	-4.23	99.16	113.12
4	D	817	MRG	C23-C22-C21	-4.06	99.71	113.12
4	L	822	2DA	C1'-N9-C4	-2.97	122.12	127.16
4	H	817	MRG	C2-N3-C4	-2.93	111.56	115.09
4	D	822	2DA	C1'-N9-C4	-2.90	122.24	127.16
4	L	817	MRG	C2-N3-C4	-2.76	111.76	115.09
4	P	822	2DA	C1'-N9-C4	-2.67	122.64	127.16
4	H	817	MRG	O3'-C3'-C2'	-2.66	101.94	110.74
4	D	817	MRG	C2-N3-C4	-2.57	111.99	115.09
4	P	817	MRG	C2-N3-C4	-2.53	112.04	115.09
4	D	817	MRG	O3'-C3'-C2'	-2.36	102.95	110.74
4	P	817	MRG	O3'-C3'-C2'	-2.09	103.81	110.74
4	H	822	2DA	C1'-N9-C4	-2.07	123.66	127.16
4	H	817	MRG	C22-C23-S24	2.01	119.52	112.45
4	L	817	MRG	C22-C23-S24	2.03	119.59	112.45
4	P	817	MRG	C22-C23-S24	2.04	119.63	112.45
4	P	817	MRG	C22-C21-N2	2.16	117.31	111.46
4	D	817	MRG	C22-C23-S24	2.24	120.32	112.45
4	L	817	MRG	C22-C21-N2	2.24	117.53	111.46
4	D	817	MRG	C22-C21-N2	2.30	117.68	111.46
4	D	817	MRG	C6-N1-C2	6.85	125.26	115.31
4	P	817	MRG	C6-N1-C2	6.86	125.28	115.31
4	H	817	MRG	C6-N1-C2	6.88	125.31	115.31
4	L	817	MRG	C6-N1-C2	6.88	125.31	115.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	817	MRG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	822	2DA	1	0
4	H	817	MRG	3	0
4	H	822	2DA	1	0
4	L	817	MRG	3	0
4	L	822	2DA	1	0
4	P	817	MRG	3	0
4	P	822	2DA	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ZP4	A	823	5	40,57,57	1.28	5 (12%)	52,88,88	2.81	9 (17%)
7	GOL	B	438	-	5,5,5	0.60	0	5,5,5	0.37	0
6	ZP4	E	823	5	40,57,57	1.21	4 (10%)	52,88,88	2.86	8 (15%)
7	GOL	F	438	-	5,5,5	0.48	0	5,5,5	0.35	0
6	ZP4	I	823	5	40,57,57	1.24	6 (15%)	52,88,88	2.82	9 (17%)
8	SWE	J	438	-	24,24,24	0.52	0	36,36,36	0.92	0
6	ZP4	M	823	5	40,57,57	1.27	5 (12%)	52,88,88	2.87	7 (13%)

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
6	ZP4	A	823	5	-	0/33/69/69	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	438	-	-	0/4/4/4	0/0/0/0
6	ZP4	E	823	5	-	0/33/69/69	0/5/5/5
7	GOL	F	438	-	-	0/4/4/4	0/0/0/0
6	ZP4	I	823	5	-	0/33/69/69	0/5/5/5
8	SWE	J	438	-	-	0/12/51/51	0/2/2/2
6	ZP4	M	823	5	-	0/33/69/69	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	823	ZP4	C6-C5	-2.71	1.32	1.40
6	A	823	ZP4	C6-C5	-2.20	1.34	1.40
6	I	823	ZP4	C6-C5	-2.11	1.34	1.40
6	E	823	ZP4	C2R-N3R	2.17	1.36	1.32
6	I	823	ZP4	C2R-N3R	2.22	1.36	1.32
6	M	823	ZP4	C2R-N3R	2.30	1.36	1.32
6	I	823	ZP4	C6-N1	2.37	1.38	1.35
6	M	823	ZP4	C6-N1	2.49	1.38	1.35
6	A	823	ZP4	C4-N3	2.52	1.37	1.33
6	A	823	ZP4	C2R-N3R	2.82	1.37	1.32
6	I	823	ZP4	O41-C11	3.03	1.45	1.41
6	I	823	ZP4	C4-N3	3.03	1.38	1.33
6	E	823	ZP4	O41-C11	3.06	1.45	1.41
6	M	823	ZP4	O41-C11	3.16	1.45	1.41
6	A	823	ZP4	O41-C11	3.16	1.45	1.41
6	M	823	ZP4	C5R-C4R	3.62	1.48	1.40
6	E	823	ZP4	C5R-C4R	3.63	1.48	1.40
6	M	823	ZP4	C4-N3	3.64	1.39	1.33
6	I	823	ZP4	C5R-C4R	3.78	1.49	1.40
6	A	823	ZP4	C5R-C4R	3.90	1.49	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	823	ZP4	C5-C4-N3	-9.19	114.90	125.14
6	E	823	ZP4	C5-C4-N3	-8.88	115.25	125.14
6	A	823	ZP4	C5-C4-N3	-8.59	115.58	125.14
6	I	823	ZP4	C5-C4-N3	-8.57	115.59	125.14
6	M	823	ZP4	N3R-C2R-N1R	-8.02	122.75	128.89
6	E	823	ZP4	N3R-C2R-N1R	-8.00	122.77	128.89
6	I	823	ZP4	N3R-C2R-N1R	-7.93	122.82	128.89
6	A	823	ZP4	N3R-C2R-N1R	-7.54	123.12	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	823	ZP4	PD-O3G-PG	-4.51	120.07	132.73
6	M	823	ZP4	PD-O3G-PG	-4.43	120.28	132.73
6	A	823	ZP4	PD-O3G-PG	-4.42	120.33	132.73
6	A	823	ZP4	PG-O3B-PB	-4.39	120.40	132.73
6	M	823	ZP4	PG-O3B-PB	-4.13	121.13	132.73
6	E	823	ZP4	PG-O3B-PB	-4.12	121.16	132.73
6	I	823	ZP4	PG-O3B-PB	-3.58	122.67	132.73
6	I	823	ZP4	PD-O3G-PG	-3.47	122.99	132.73
6	A	823	ZP4	C4R-C5R-N7R	-3.45	106.31	109.48
6	E	823	ZP4	C4R-C5R-N7R	-3.30	106.44	109.48
6	I	823	ZP4	C4R-C5R-N7R	-3.23	106.51	109.48
6	M	823	ZP4	C4R-C5R-N7R	-3.12	106.61	109.48
6	A	823	ZP4	PB-O3A-PA	-2.51	125.69	132.73
6	E	823	ZP4	PB-O3A-PA	-2.13	126.76	132.73
6	I	823	ZP4	C21-C11-N9R	-2.09	111.11	114.29
6	A	823	ZP4	O41-C11-N9R	2.00	112.29	108.10
6	E	823	ZP4	C2R-N1R-C6R	2.02	122.38	118.77
6	M	823	ZP4	C5A-C5-C6	2.08	122.80	118.62
6	I	823	ZP4	C5A-C5-C6	2.28	123.21	118.62
6	A	823	ZP4	C5A-C5-C6	2.33	123.30	118.62
6	I	823	ZP4	O41-C11-N9R	2.94	114.25	108.10
6	A	823	ZP4	C4-N3-C2	13.49	126.91	115.25
6	E	823	ZP4	C4-N3-C2	13.77	127.15	115.25
6	I	823	ZP4	C4-N3-C2	13.78	127.16	115.25
6	M	823	ZP4	C4-N3-C2	13.93	127.29	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	823	ZP4	10	0
6	E	823	ZP4	9	0
6	I	823	ZP4	4	0
8	J	438	SWE	5	0
6	M	823	ZP4	7	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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	560/562 (99%)	0.19	8 (1%) 78 65	31, 60, 76, 87	0
1	E	560/562 (99%)	0.21	8 (1%) 78 65	35, 62, 78, 88	0
1	I	560/562 (99%)	0.86	92 (16%) 2 1	100, 115, 121, 124	0
1	M	560/562 (99%)	1.78	197 (35%) 0 0	109, 129, 134, 137	0
2	B	425/437 (97%)	0.35	15 (3%) 48 32	22, 54, 84, 97	0
2	F	419/437 (95%)	0.33	15 (3%) 46 31	29, 58, 84, 91	0
2	J	419/437 (95%)	1.13	94 (22%) 1 1	102, 115, 121, 126	0
2	N	419/437 (95%)	2.12	172 (41%) 0 0	117, 129, 133, 137	0
3	C	25/27 (92%)	-0.04	0 100 100	29, 62, 82, 92	0
3	G	25/27 (92%)	-0.11	0 100 100	32, 65, 84, 89	0
3	K	25/27 (92%)	-0.29	0 100 100	111, 117, 123, 125	0
3	O	25/27 (92%)	0.74	5 (20%) 1 1	127, 130, 135, 139	0
4	D	19/21 (90%)	-0.04	0 100 100	40, 58, 87, 89	0
4	H	19/21 (90%)	-0.10	0 100 100	42, 62, 88, 96	0
4	L	19/21 (90%)	-0.06	1 (5%) 30 17	105, 115, 123, 123	0
4	P	19/21 (90%)	0.46	2 (10%) 8 5	124, 131, 134, 134	0
All	All	4098/4188 (97%)	0.82	609 (14%) 3 2	22, 94, 131, 139	0

All (609) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	325	LEU	15.5
2	N	21	VAL	13.4
2	N	108	VAL	11.3
2	N	159	ILE	11.2
2	N	3	SER	10.7

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Mol	Chain	Res	Type	RSRZ
2	J	360	ALA	10.5
2	N	10	VAL	10.3
1	M	252	TRP	9.8
1	M	368	LEU	9.7
2	N	107	THR	9.7
1	M	112	GLY	9.6
1	M	114	ALA	9.5
1	M	149	LEU	9.4
1	I	1	PRO	9.4
2	J	220	LYS	8.9
2	J	231	GLY	8.9
1	M	26	LEU	8.8
2	N	18	GLY	8.5
2	N	9	PRO	8.4
2	N	111	VAL	8.4
1	M	131	THR	8.2
1	M	132	ILE	8.1
2	N	429	GLY	8.1
2	F	67	ASP	8.1
2	N	221	HIS	7.9
2	J	221	HIS	7.9
2	N	109	LEU	7.8
1	M	75	VAL	7.8
2	N	409	THR	7.8
2	N	212	TRP	7.7
2	N	8	VAL	7.6
1	I	560	LEU	7.5
2	N	147	ASN	7.3
2	J	61	PHE	7.3
1	M	187	LEU	7.3
2	N	161	GLN	7.3
2	N	130	PHE	7.2
1	M	50	ILE	7.1
1	M	17	ASP	7.1
1	M	21	VAL	7.1
2	N	219	LYS	6.9
2	N	211	ARG	6.9
1	M	113	ASP	6.9
2	N	54	ASN	6.8
2	N	389	PHE	6.7
2	N	145	GLN	6.7
1	M	96	HIS	6.6

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Mol	Chain	Res	Type	RSRZ
1	M	115	TYR	6.6
1	M	67	ASN	6.6
2	J	361	HIS	6.6
3	O	704	DC	6.5
1	A	560	LEU	6.5
2	N	95	PRO	6.5
2	N	324	ASP	6.5
2	J	7	THR	6.4
1	M	12	LEU	6.3
1	M	269	GLN	6.3
2	N	76	ASP	6.3
2	N	207	GLN	6.3
1	M	150	PRO	6.3
1	I	19	PRO	6.2
1	M	55	PRO	6.2
2	B	431	HIS	6.1
1	M	63	ILE	6.1
1	M	116	PHE	6.1
1	M	19	PRO	6.1
2	N	355	ALA	6.0
1	M	273	GLY	5.9
1	M	246	LEU	5.8
2	N	178	ILE	5.8
2	N	160	PHE	5.7
2	N	117	SER	5.7
1	M	325	LEU	5.6
1	M	363	ASN	5.6
1	M	366	LYS	5.6
2	N	68	SER	5.6
2	N	127	TYR	5.6
1	M	84	THR	5.6
2	N	71	TRP	5.6
1	I	149	LEU	5.5
1	M	212	TRP	5.5
1	M	168	LEU	5.5
2	N	7	THR	5.5
2	N	218	ASP	5.5
1	M	3	SER	5.5
1	I	118	VAL	5.5
1	M	186	ASP	5.5
1	I	5	ILE	5.4
1	I	246	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
2	N	192	ASP	5.4
1	M	38	CYS	5.3
1	M	247	PRO	5.3
2	J	207	GLN	5.3
2	N	56	TYR	5.3
2	N	195	ILE	5.2
2	J	93	GLY	5.1
1	M	214	LEU	5.1
1	M	306	ASN	5.1
1	M	34	LEU	5.1
1	M	412	PRO	5.1
1	M	276	VAL	5.1
2	N	12	LEU	5.1
2	N	124	PHE	5.0
2	N	246	LEU	5.0
2	J	68	SER	5.0
1	E	1	PRO	5.0
2	J	107	THR	5.0
2	J	67	ASP	5.0
1	M	135	ILE	5.0
2	N	146	TYR	5.0
1	M	25	PRO	5.0
1	M	111	VAL	5.0
1	M	174	GLN	5.0
1	M	365	VAL	4.9
2	F	314	VAL	4.9
2	N	17	ASP	4.9
2	B	360	ALA	4.9
1	M	245	VAL	4.9
2	N	110	ASP	4.9
1	M	389	PHE	4.8
1	E	559	VAL	4.8
2	N	134	SER	4.8
1	M	249	LYS	4.8
2	J	159	ILE	4.8
2	J	97	PRO	4.8
2	J	146	TYR	4.8
1	M	117	SER	4.8
2	J	161	GLN	4.8
2	N	11	LYS	4.8
2	J	164	MET	4.7
2	N	62	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	26	LEU	4.7
2	J	3	SER	4.7
2	B	67	ASP	4.7
1	M	71	TRP	4.6
2	N	408	ALA	4.6
2	J	88	TRP	4.6
1	M	244	ILE	4.6
1	M	205	LEU	4.5
1	M	279	LEU	4.5
2	J	359	GLY	4.5
1	M	275	LYS	4.5
1	M	314	VAL	4.5
2	N	216	THR	4.5
2	N	164	MET	4.5
2	N	215	THR	4.5
2	J	222	GLN	4.5
1	M	397	THR	4.5
1	M	302	GLU	4.4
2	B	359	GLY	4.4
1	I	114	ALA	4.4
1	I	252	TRP	4.4
1	M	423	VAL	4.4
1	M	60	VAL	4.4
1	M	20	LYS	4.4
2	N	150	PRO	4.4
1	M	136	ASN	4.4
1	I	130	PHE	4.3
1	M	290	THR	4.3
2	N	197	GLN	4.3
2	N	133	PRO	4.3
1	I	73	LYS	4.3
2	J	95	PRO	4.3
1	M	388	LYS	4.3
1	I	293	ILE	4.3
1	M	122	GLU	4.2
1	I	342	TYR	4.2
2	N	335	GLY	4.2
1	I	195	ILE	4.2
1	E	2	ILE	4.2
2	N	39	THR	4.2
1	M	237	ASP	4.2
2	N	131	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	88	TRP	4.2
2	N	151	GLN	4.1
2	N	191	SER	4.1
2	N	67	ASP	4.1
2	N	220	LYS	4.1
1	M	335	GLY	4.1
1	M	354	TYR	4.1
1	M	68	SER	4.1
1	I	66	LYS	4.1
2	F	360	ALA	4.1
1	M	251	SER	4.1
2	N	203	GLU	4.1
1	I	18	GLY	4.1
2	N	52	PRO	4.1
2	N	383	TRP	4.1
1	I	288	ALA	4.1
1	M	324	ASP	4.0
1	M	408	ALA	4.0
1	M	56	TYR	4.0
1	E	68	SER	4.0
1	I	188	TYR	4.0
1	I	295	LEU	4.0
1	M	54	ASN	4.0
1	M	196	GLY	4.0
2	B	434	HIS	4.0
1	M	27	THR	4.0
2	N	334	GLN	4.0
1	M	192	ASP	4.0
2	N	128	THR	4.0
1	M	14	PRO	4.0
2	N	204	GLU	3.9
1	I	192	ASP	3.9
2	N	292	VAL	3.9
1	I	303	LEU	3.9
2	J	215	THR	3.9
2	N	158	ALA	3.9
2	N	270	ILE	3.9
2	N	75	VAL	3.9
2	B	358	ARG	3.9
2	N	323	LYS	3.8
2	J	288	ALA	3.8
1	E	560	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	N	28	GLU	3.8
2	F	231	GLY	3.8
2	J	144	TYR	3.8
2	N	239	TRP	3.8
2	J	160	PHE	3.8
2	N	182	GLN	3.8
2	N	368	LEU	3.8
1	M	11	LYS	3.8
2	F	359	GLY	3.8
2	J	168	LEU	3.8
2	J	145	GLN	3.8
2	J	219	LYS	3.8
2	N	140	PRO	3.7
1	M	146	TYR	3.7
2	N	30	LYS	3.7
1	M	151	GLN	3.7
2	N	180	ILE	3.7
2	N	176	PRO	3.7
1	I	60	VAL	3.7
2	N	410	TRP	3.7
2	B	3	SER	3.7
2	J	274	ILE	3.7
1	M	455	ALA	3.7
2	N	401	TRP	3.7
2	N	343	GLN	3.6
1	M	8	VAL	3.6
2	N	115	TYR	3.6
1	I	275	LYS	3.6
2	N	25	PRO	3.6
2	N	244	ILE	3.6
1	I	128	THR	3.6
2	J	5	ILE	3.5
1	M	283	LEU	3.5
2	F	358	ARG	3.5
3	O	703	DG	3.5
2	N	199	ARG	3.5
2	N	319	TYR	3.5
1	I	135	ILE	3.5
1	I	55	PRO	3.5
1	M	313	PRO	3.5
1	I	132	ILE	3.5
2	N	348	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	187	LEU	3.4
2	N	375	ILE	3.4
1	M	169	GLU	3.4
1	A	1	PRO	3.4
1	M	340	GLN	3.4
1	M	502	ALA	3.4
1	I	325	LEU	3.4
2	N	356	ARG	3.4
1	M	175	ASN	3.4
2	N	232	TYR	3.4
1	M	57	ASN	3.4
1	M	127	TYR	3.3
1	M	188	TYR	3.3
2	F	315	HIS	3.3
2	N	59	PRO	3.3
2	N	293	ILE	3.3
1	A	455	ALA	3.3
2	N	53	GLU	3.3
1	I	271	TYR	3.3
1	I	455	ALA	3.3
1	M	506	ILE	3.3
1	M	271	TYR	3.2
1	I	102	LYS	3.2
1	M	23	GLN	3.2
1	M	207	GLN	3.2
2	J	182	GLN	3.2
2	J	10	VAL	3.2
2	J	4	PRO	3.2
1	M	410	TRP	3.2
1	I	17	ASP	3.2
1	I	116	PHE	3.2
1	M	18	GLY	3.2
2	J	92	LEU	3.2
2	J	87	PHE	3.2
1	I	20	LYS	3.2
2	F	283	LEU	3.2
2	N	38	CYS	3.2
2	J	409	THR	3.2
2	B	432	HIS	3.2
1	I	146	TYR	3.2
1	M	524	GLN	3.2
1	M	4	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	297	GLU	3.2
1	M	241	VAL	3.2
2	N	61	PHE	3.2
1	I	171	PHE	3.1
1	I	456	GLY	3.1
1	I	72	ARG	3.1
2	N	260	LEU	3.1
1	I	247	PRO	3.1
1	M	180	ILE	3.1
1	M	293	ILE	3.1
2	N	63	ILE	3.1
2	N	391	LEU	3.1
1	M	37	ILE	3.1
2	N	327	ALA	3.1
2	J	233	GLU	3.1
2	J	76	ASP	3.1
3	O	705	DA	3.1
2	N	129	ALA	3.1
1	I	141	GLY	3.1
1	M	106	VAL	3.1
2	N	242	GLN	3.1
2	N	346	PHE	3.1
2	N	349	LEU	3.1
2	N	264	LEU	3.1
2	J	124	PHE	3.1
2	N	210	LEU	3.1
2	J	141	GLY	3.0
1	M	413	GLU	3.0
1	M	511	ASP	3.0
1	I	168	LEU	3.0
1	I	199	ARG	3.0
2	J	187	LEU	3.0
2	J	106	VAL	3.0
2	J	241	VAL	3.0
1	M	288	ALA	3.0
2	J	246	LEU	3.0
1	M	406	TRP	3.0
1	I	194	GLU	3.0
2	J	17	ASP	3.0
1	M	5	ILE	3.0
1	M	248	GLU	3.0
1	M	209	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	189	VAL	3.0
1	I	205	LEU	2.9
1	M	208	HIS	2.9
2	N	231	GLY	2.9
1	I	279	LEU	2.9
1	I	282	LEU	2.9
1	M	189	VAL	2.9
1	I	58	THR	2.9
1	I	52	PRO	2.9
1	M	261	VAL	2.9
2	N	163	SER	2.9
1	I	75	VAL	2.9
1	M	173	LYS	2.9
2	J	214	LEU	2.9
2	N	37	ILE	2.9
1	I	164	MET	2.9
1	I	332	GLN	2.9
1	M	9	PRO	2.9
2	N	222	GLN	2.9
1	M	48	SER	2.9
1	M	223	LYS	2.9
1	I	53	GLU	2.9
1	M	274	ILE	2.9
1	M	66	LYS	2.9
1	M	530	LYS	2.9
2	N	411	ILE	2.8
2	J	389	PHE	2.8
1	M	222	GLN	2.8
2	F	3	SER	2.8
2	N	416	PHE	2.8
1	M	33	ALA	2.8
1	M	503	LEU	2.8
1	I	68	SER	2.8
2	N	243	PRO	2.8
2	N	149	LEU	2.8
2	J	96	HIS	2.8
1	M	496	VAL	2.8
1	M	272	PRO	2.8
2	B	266	TRP	2.8
2	N	248	GLU	2.8
1	M	171	PHE	2.8
1	M	65	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	559	VAL	2.8
2	N	114	ALA	2.8
1	M	469	LEU	2.7
1	M	49	LYS	2.7
1	M	218	ASP	2.7
1	M	299	ALA	2.7
2	N	362	THR	2.7
2	J	157	PRO	2.7
2	J	216	THR	2.7
2	J	422	LEU	2.7
1	I	48	SER	2.7
1	I	8	VAL	2.7
2	J	166	LYS	2.7
1	I	214	LEU	2.7
2	N	102	LYS	2.7
1	I	34	LEU	2.7
1	M	377	THR	2.7
1	M	281	LYS	2.7
1	M	250	ASP	2.7
2	N	200	THR	2.7
1	M	452	LEU	2.7
2	N	353	LYS	2.7
2	J	152	GLY	2.6
1	M	200	THR	2.6
1	I	144	TYR	2.6
1	I	248	GLU	2.6
2	N	358	ARG	2.6
1	E	222	GLN	2.6
2	J	232	TYR	2.6
1	M	292	VAL	2.6
2	J	111	VAL	2.6
1	M	159	ILE	2.6
2	N	354	TYR	2.6
1	M	421	PRO	2.6
2	J	110	ASP	2.6
2	J	211	ARG	2.6
1	I	133	PRO	2.6
2	N	157	PRO	2.6
1	M	90	VAL	2.6
1	M	291	GLU	2.6
1	I	304	ALA	2.6
2	J	60	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	355	ALA	2.6
2	N	13	LYS	2.6
2	N	97	PRO	2.6
1	M	72	ARG	2.6
1	M	534	ALA	2.6
2	J	358	ARG	2.5
2	N	148	VAL	2.5
2	N	16	MET	2.5
1	M	371	ALA	2.5
1	M	301	LEU	2.5
1	M	453	GLY	2.5
1	M	118	VAL	2.5
1	A	456	GLY	2.5
1	M	286	THR	2.5
2	N	90	VAL	2.5
2	J	16	MET	2.5
2	J	343	GLN	2.5
1	I	428	GLN	2.5
1	M	77	PHE	2.5
2	F	425	LEU	2.5
2	B	238	LYS	2.5
1	I	525	LEU	2.5
2	F	246	LEU	2.5
4	L	802	DA	2.5
1	E	359	GLY	2.5
1	I	388	LYS	2.5
2	J	244	ILE	2.5
1	I	222	GLN	2.5
2	J	336	GLN	2.5
2	N	414	TRP	2.5
2	N	388	LYS	2.5
1	M	392	PRO	2.5
2	J	282	LEU	2.5
4	P	814	DC	2.5
1	M	15	GLY	2.5
2	B	357	MET	2.5
2	N	86	ASP	2.5
2	N	135	ILE	2.4
1	I	354	TYR	2.4
2	N	4	PRO	2.4
2	N	93	GLY	2.4
2	N	177	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	500	GLN	2.4
2	J	8	VAL	2.4
1	I	136	ASN	2.4
2	N	66	LYS	2.4
2	N	208	HIS	2.4
2	N	298	GLU	2.4
2	J	209	LEU	2.4
2	J	391	LEU	2.4
1	M	145	GLN	2.4
1	M	124	PHE	2.4
1	M	178	ILE	2.4
2	N	183	TYR	2.4
1	I	551	LEU	2.4
1	I	559	VAL	2.4
2	J	250	ASP	2.4
2	N	361	HIS	2.4
2	F	242	GLN	2.4
2	N	118	VAL	2.4
2	N	187	LEU	2.4
2	J	384	GLY	2.4
2	J	260	LEU	2.4
1	M	409	THR	2.4
1	I	398	TRP	2.4
2	J	178	ILE	2.4
1	I	134	SER	2.3
1	I	14	PRO	2.3
2	B	430	GLY	2.3
1	I	274	ILE	2.3
1	M	160	PHE	2.3
1	I	50	ILE	2.3
1	I	142	ILE	2.3
3	O	717	DC	2.3
1	I	2	ILE	2.3
1	M	144	TYR	2.3
1	M	337	TRP	2.3
2	B	435	HIS	2.3
1	I	209	LEU	2.3
1	M	327	ALA	2.3
2	N	168	LEU	2.3
2	N	282	LEU	2.3
2	J	329	ILE	2.3
4	P	820	DC	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	69	THR	2.3
2	N	35	VAL	2.3
1	M	277	ARG	2.3
2	N	196	GLY	2.3
1	M	243	PRO	2.3
1	M	396	GLU	2.3
1	M	176	PRO	2.3
2	B	246	LEU	2.3
2	J	239	TRP	2.3
1	A	545	ASN	2.2
1	I	308	GLU	2.2
1	I	51	GLY	2.2
1	M	315	HIS	2.2
2	N	106	VAL	2.2
2	J	174	GLN	2.2
2	N	91	GLN	2.2
2	F	429	GLY	2.2
1	M	482	ILE	2.2
2	J	85	GLN	2.2
2	J	327	ALA	2.2
1	A	434	ILE	2.2
1	M	326	ILE	2.2
1	M	323	LYS	2.2
2	N	201	LYS	2.2
2	N	267	ALA	2.2
1	A	214	LEU	2.2
2	N	252	TRP	2.2
1	I	312	GLU	2.2
1	M	95	PRO	2.2
1	M	422	LEU	2.2
1	M	310	LEU	2.2
2	F	361	HIS	2.2
2	N	271	TYR	2.2
1	M	270	ILE	2.2
2	N	278	GLN	2.2
2	N	214	LEU	2.2
2	N	64	LYS	2.1
1	I	100	LEU	2.1
1	M	419	THR	2.1
1	I	233	GLU	2.1
2	J	192	ASP	2.1
2	N	198	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	205	LEU	2.1
2	J	249	LYS	2.1
1	M	346	PHE	2.1
1	M	233	GLU	2.1
1	M	238	LYS	2.1
1	M	345	PRO	2.1
2	J	341	ILE	2.1
1	I	124	PHE	2.1
2	N	193	LEU	2.1
1	M	42	GLU	2.1
2	J	163	SER	2.1
1	E	467	VAL	2.1
2	J	42	GLU	2.1
2	N	142	ILE	2.1
1	I	115	TYR	2.1
2	N	22	LYS	2.1
2	J	218	ASP	2.1
2	N	341	ILE	2.1
2	J	54	ASN	2.1
2	N	233	GLU	2.1
2	N	378	GLU	2.1
1	M	181	TYR	2.1
1	M	260	LEU	2.1
2	J	170	PRO	2.1
2	N	181	TYR	2.1
1	M	76	ASP	2.1
2	N	84	THR	2.1
2	N	174	GLN	2.1
1	M	479	LEU	2.1
2	F	187	LEU	2.1
2	N	112	GLY	2.1
1	I	3	SER	2.1
1	M	105	SER	2.1
1	M	163	SER	2.1
2	J	105	SER	2.1
1	M	341	ILE	2.1
1	M	507	GLN	2.1
1	M	383	TRP	2.1
2	J	257	ILE	2.1
1	I	137	ASN	2.1
2	J	346	PHE	2.1
1	M	24	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	80	LEU	2.0
2	J	323	LYS	2.0
2	N	288	ALA	2.0
2	J	108	VAL	2.0
2	B	214	LEU	2.0
1	M	102	LYS	2.0
1	M	147	ASN	2.0
1	I	140	PRO	2.0
1	M	486	LEU	2.0
2	J	217	PRO	2.0
1	M	219	GLN	2.0
1	M	435	VAL	2.0
2	N	46	LYS	2.0
1	I	178	ILE	2.0
3	O	712	DC	2.0
1	I	425	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	MRG	D	817	26/27	0.96	0.24	-	46,51,54,55	0
4	2DA	D	822	20/21	0.96	0.22	-	41,45,48,50	0
4	MRG	L	817	26/27	0.79	0.20	-	117,120,123,124	0
4	MRG	H	817	26/27	0.95	0.21	-	49,55,62,63	0
4	2DA	P	822	20/21	0.46	0.37	-	131,132,133,133	0
4	MRG	P	817	26/27	0.76	0.16	-	125,132,138,143	0
4	2DA	H	822	20/21	0.96	0.21	-	46,52,61,61	0
4	2DA	L	822	20/21	0.90	0.18	-	112,114,115,115	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
7	GOL	B	438	6/6	0.79	0.37	2.67	61,65,67,67	0
5	MG	M	602	1/1	0.82	0.29	0.53	94,94,94,94	0
5	MG	E	602	1/1	0.95	0.22	0.40	13,13,13,13	0
5	MG	E	600	1/1	0.99	0.21	0.38	28,28,28,28	0
6	ZP4	A	823	53/53	0.92	0.27	0.17	45,69,92,94	0
6	ZP4	E	823	53/53	0.91	0.25	0.14	50,75,91,94	0
5	MG	I	600	1/1	0.96	0.26	-0.28	96,96,96,96	0
6	ZP4	I	823	53/53	0.89	0.19	-0.72	107,121,125,126	0
6	ZP4	M	823	53/53	0.71	0.27	-0.82	128,135,138,139	0
8	SWE	J	438	23/23	0.77	0.21	-1.00	94,99,100,101	0
5	MG	I	602	1/1	0.96	0.19	-1.07	64,64,64,64	0
5	MG	A	602	1/1	0.95	0.15	-1.42	24,24,24,24	0
5	MG	M	600	1/1	0.42	0.15	-1.53	123,123,123,123	0
5	MG	A	600	1/1	0.97	0.18	-3.16	27,27,27,27	0
7	GOL	F	438	6/6	0.68	0.28	-	69,71,73,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.