



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:59 AM GMT

PDB ID : 3GLI  
Title : Crystal Structure of the E. coli clamp loader bound to Primer-Template DNA and Psi Peptide  
Authors : Simonetta, K.R.; Cantor, A.J.; Kuriyan, J.  
Deposited on : 2009-03-12  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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:

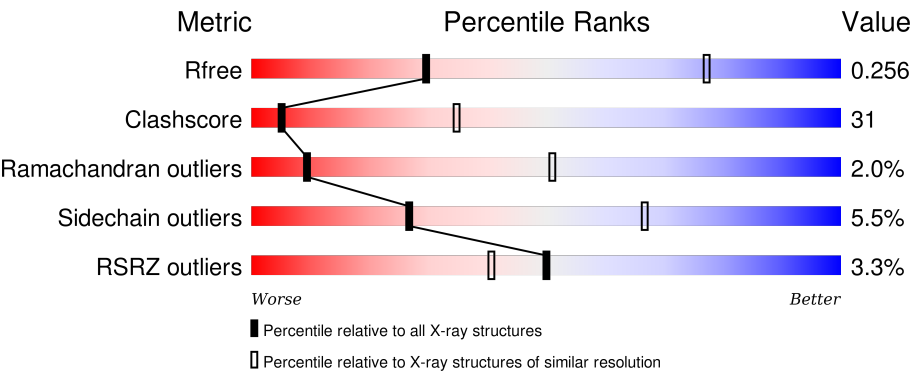
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	343	<div><div>11%</div><div>48%</div><div>45%</div><div>• •</div></div>
1	F	343	<div><div>14%</div><div>45%</div><div>48%</div><div>• •</div></div>
2	B	395	<div><div>50%</div><div>36%</div><div>•</div><div>9%</div></div>
2	C	395	<div><div>47%</div><div>41%</div><div>5%</div><div>8%</div></div>
2	D	395	<div><div>%</div><div>44%</div><div>44%</div><div>•</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	395	
2	H	395	
2	I	395	
3	E	334	
3	J	334	
4	K	15	
4	M	15	
5	L	10	
5	N	10	
6	O	27	
6	P	27	

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
9	MG	B	412	-	-	-	X
9	MG	H	416	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29139 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			
1	F	334	Total	C	N	O	S	0	0	0
			2659	1684	484	481	10			

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	0	0
			2791	1753	506	516	16			
2	C	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	D	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			
2	G	373	Total	C	N	O	S	0	0	0
			2903	1826	524	536	17			
2	H	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	I	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	EXPRESSION TAG	UNP P06710
B	-20	GLY	-	EXPRESSION TAG	UNP P06710
B	-19	SER	-	EXPRESSION TAG	UNP P06710
B	-18	SER	-	EXPRESSION TAG	UNP P06710
B	-17	HIS	-	EXPRESSION TAG	UNP P06710
B	-16	HIS	-	EXPRESSION TAG	UNP P06710
B	-15	HIS	-	EXPRESSION TAG	UNP P06710
B	-14	HIS	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	EXPRESSION TAG	UNP P06710
B	-12	HIS	-	EXPRESSION TAG	UNP P06710
B	-11	SER	-	EXPRESSION TAG	UNP P06710
B	-10	SER	-	EXPRESSION TAG	UNP P06710
B	-9	GLY	-	EXPRESSION TAG	UNP P06710
B	-8	LEU	-	EXPRESSION TAG	UNP P06710
B	-7	GLU	-	EXPRESSION TAG	UNP P06710
B	-6	VAL	-	EXPRESSION TAG	UNP P06710
B	-5	LEU	-	EXPRESSION TAG	UNP P06710
B	-4	PHE	-	EXPRESSION TAG	UNP P06710
B	-3	GLN	-	EXPRESSION TAG	UNP P06710
B	-2	GLY	-	EXPRESSION TAG	UNP P06710
B	-1	PRO	-	EXPRESSION TAG	UNP P06710
B	0	HIS	-	EXPRESSION TAG	UNP P06710
C	-21	MET	-	EXPRESSION TAG	UNP P06710
C	-20	GLY	-	EXPRESSION TAG	UNP P06710
C	-19	SER	-	EXPRESSION TAG	UNP P06710
C	-18	SER	-	EXPRESSION TAG	UNP P06710
C	-17	HIS	-	EXPRESSION TAG	UNP P06710
C	-16	HIS	-	EXPRESSION TAG	UNP P06710
C	-15	HIS	-	EXPRESSION TAG	UNP P06710
C	-14	HIS	-	EXPRESSION TAG	UNP P06710
C	-13	HIS	-	EXPRESSION TAG	UNP P06710
C	-12	HIS	-	EXPRESSION TAG	UNP P06710
C	-11	SER	-	EXPRESSION TAG	UNP P06710
C	-10	SER	-	EXPRESSION TAG	UNP P06710
C	-9	GLY	-	EXPRESSION TAG	UNP P06710
C	-8	LEU	-	EXPRESSION TAG	UNP P06710
C	-7	GLU	-	EXPRESSION TAG	UNP P06710
C	-6	VAL	-	EXPRESSION TAG	UNP P06710
C	-5	LEU	-	EXPRESSION TAG	UNP P06710
C	-4	PHE	-	EXPRESSION TAG	UNP P06710
C	-3	GLN	-	EXPRESSION TAG	UNP P06710
C	-2	GLY	-	EXPRESSION TAG	UNP P06710
C	-1	PRO	-	EXPRESSION TAG	UNP P06710
C	0	HIS	-	EXPRESSION TAG	UNP P06710
D	-21	MET	-	EXPRESSION TAG	UNP P06710
D	-20	GLY	-	EXPRESSION TAG	UNP P06710
D	-19	SER	-	EXPRESSION TAG	UNP P06710
D	-18	SER	-	EXPRESSION TAG	UNP P06710
D	-17	HIS	-	EXPRESSION TAG	UNP P06710
D	-16	HIS	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	EXPRESSION TAG	UNP P06710
D	-14	HIS	-	EXPRESSION TAG	UNP P06710
D	-13	HIS	-	EXPRESSION TAG	UNP P06710
D	-12	HIS	-	EXPRESSION TAG	UNP P06710
D	-11	SER	-	EXPRESSION TAG	UNP P06710
D	-10	SER	-	EXPRESSION TAG	UNP P06710
D	-9	GLY	-	EXPRESSION TAG	UNP P06710
D	-8	LEU	-	EXPRESSION TAG	UNP P06710
D	-7	GLU	-	EXPRESSION TAG	UNP P06710
D	-6	VAL	-	EXPRESSION TAG	UNP P06710
D	-5	LEU	-	EXPRESSION TAG	UNP P06710
D	-4	PHE	-	EXPRESSION TAG	UNP P06710
D	-3	GLN	-	EXPRESSION TAG	UNP P06710
D	-2	GLY	-	EXPRESSION TAG	UNP P06710
D	-1	PRO	-	EXPRESSION TAG	UNP P06710
D	0	HIS	-	EXPRESSION TAG	UNP P06710
G	-21	MET	-	EXPRESSION TAG	UNP P06710
G	-20	GLY	-	EXPRESSION TAG	UNP P06710
G	-19	SER	-	EXPRESSION TAG	UNP P06710
G	-18	SER	-	EXPRESSION TAG	UNP P06710
G	-17	HIS	-	EXPRESSION TAG	UNP P06710
G	-16	HIS	-	EXPRESSION TAG	UNP P06710
G	-15	HIS	-	EXPRESSION TAG	UNP P06710
G	-14	HIS	-	EXPRESSION TAG	UNP P06710
G	-13	HIS	-	EXPRESSION TAG	UNP P06710
G	-12	HIS	-	EXPRESSION TAG	UNP P06710
G	-11	SER	-	EXPRESSION TAG	UNP P06710
G	-10	SER	-	EXPRESSION TAG	UNP P06710
G	-9	GLY	-	EXPRESSION TAG	UNP P06710
G	-8	LEU	-	EXPRESSION TAG	UNP P06710
G	-7	GLU	-	EXPRESSION TAG	UNP P06710
G	-6	VAL	-	EXPRESSION TAG	UNP P06710
G	-5	LEU	-	EXPRESSION TAG	UNP P06710
G	-4	PHE	-	EXPRESSION TAG	UNP P06710
G	-3	GLN	-	EXPRESSION TAG	UNP P06710
G	-2	GLY	-	EXPRESSION TAG	UNP P06710
G	-1	PRO	-	EXPRESSION TAG	UNP P06710
G	0	HIS	-	EXPRESSION TAG	UNP P06710
H	-21	MET	-	EXPRESSION TAG	UNP P06710
H	-20	GLY	-	EXPRESSION TAG	UNP P06710
H	-19	SER	-	EXPRESSION TAG	UNP P06710
H	-18	SER	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	EXPRESSION TAG	UNP P06710
H	-16	HIS	-	EXPRESSION TAG	UNP P06710
H	-15	HIS	-	EXPRESSION TAG	UNP P06710
H	-14	HIS	-	EXPRESSION TAG	UNP P06710
H	-13	HIS	-	EXPRESSION TAG	UNP P06710
H	-12	HIS	-	EXPRESSION TAG	UNP P06710
H	-11	SER	-	EXPRESSION TAG	UNP P06710
H	-10	SER	-	EXPRESSION TAG	UNP P06710
H	-9	GLY	-	EXPRESSION TAG	UNP P06710
H	-8	LEU	-	EXPRESSION TAG	UNP P06710
H	-7	GLU	-	EXPRESSION TAG	UNP P06710
H	-6	VAL	-	EXPRESSION TAG	UNP P06710
H	-5	LEU	-	EXPRESSION TAG	UNP P06710
H	-4	PHE	-	EXPRESSION TAG	UNP P06710
H	-3	GLN	-	EXPRESSION TAG	UNP P06710
H	-2	GLY	-	EXPRESSION TAG	UNP P06710
H	-1	PRO	-	EXPRESSION TAG	UNP P06710
H	0	HIS	-	EXPRESSION TAG	UNP P06710
I	-21	MET	-	EXPRESSION TAG	UNP P06710
I	-20	GLY	-	EXPRESSION TAG	UNP P06710
I	-19	SER	-	EXPRESSION TAG	UNP P06710
I	-18	SER	-	EXPRESSION TAG	UNP P06710
I	-17	HIS	-	EXPRESSION TAG	UNP P06710
I	-16	HIS	-	EXPRESSION TAG	UNP P06710
I	-15	HIS	-	EXPRESSION TAG	UNP P06710
I	-14	HIS	-	EXPRESSION TAG	UNP P06710
I	-13	HIS	-	EXPRESSION TAG	UNP P06710
I	-12	HIS	-	EXPRESSION TAG	UNP P06710
I	-11	SER	-	EXPRESSION TAG	UNP P06710
I	-10	SER	-	EXPRESSION TAG	UNP P06710
I	-9	GLY	-	EXPRESSION TAG	UNP P06710
I	-8	LEU	-	EXPRESSION TAG	UNP P06710
I	-7	GLU	-	EXPRESSION TAG	UNP P06710
I	-6	VAL	-	EXPRESSION TAG	UNP P06710
I	-5	LEU	-	EXPRESSION TAG	UNP P06710
I	-4	PHE	-	EXPRESSION TAG	UNP P06710
I	-3	GLN	-	EXPRESSION TAG	UNP P06710
I	-2	GLY	-	EXPRESSION TAG	UNP P06710
I	-1	PRO	-	EXPRESSION TAG	UNP P06710
I	0	HIS	-	EXPRESSION TAG	UNP P06710

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			
3	J	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			
4	M	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*AP\*TP\*A)-3').

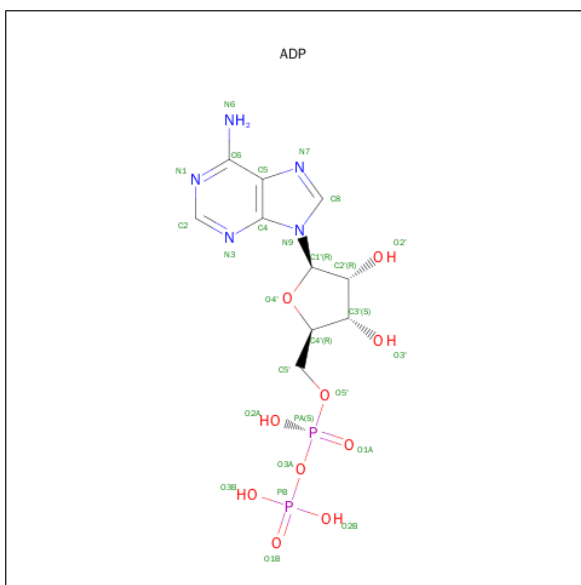
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is a protein called DNA polymerase III subunit psi.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	27	Total	C	N	O	0	0	0
			224	138	46	40			
6	P	27	Total	C	N	O	0	0	0
			224	138	46	40			

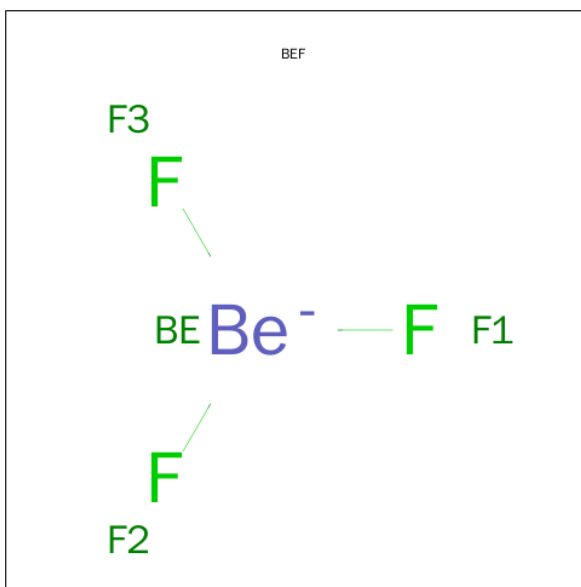
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	I	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $\text{BeF}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Be	F	0	0
			4	1	3		
8	C	1	Total	Be	F	0	0
			4	1	3		
8	D	1	Total	Be	F	0	0
			4	1	3		
8	G	1	Total	Be	F	0	0
			4	1	3		
8	H	1	Total	Be	F	0	0
			4	1	3		
8	I	1	Total	Be	F	0	0
			4	1	3		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		
9	H	1	Total	Mg	0	0
			1	1		
9	B	1	Total	Mg	0	0
			1	1		
9	I	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

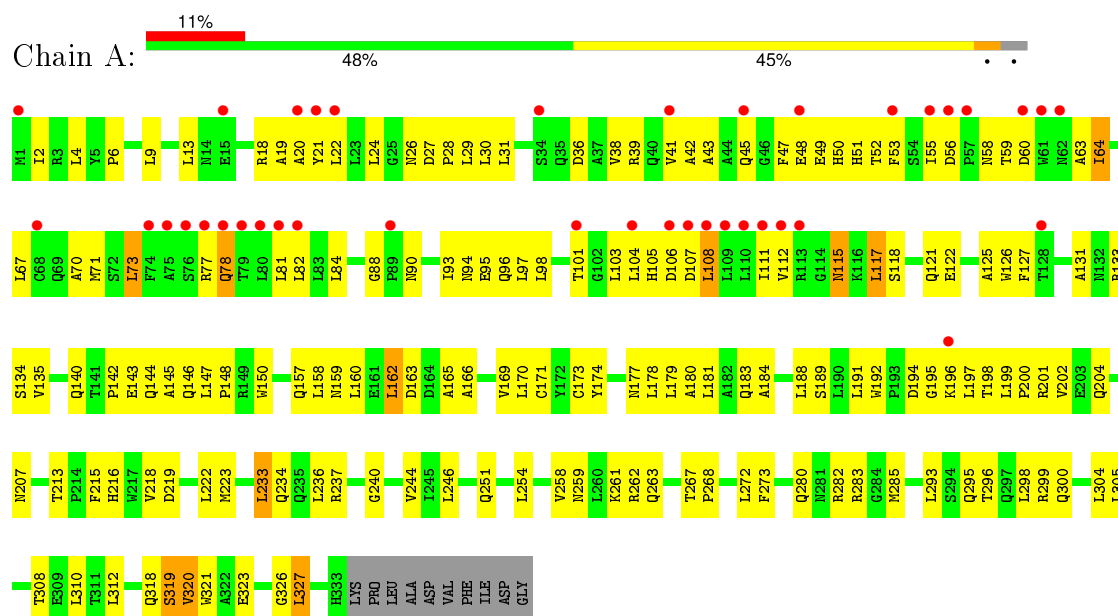
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	1	Total 1	Zn 1	0	0
10	J	1	Total 1	Zn 1	0	0
10	D	1	Total 1	Zn 1	0	0
10	E	1	Total 1	Zn 1	0	0
10	H	1	Total 1	Zn 1	0	0
10	B	1	Total 1	Zn 1	0	0
10	I	1	Total 1	Zn 1	0	0
10	C	1	Total 1	Zn 1	0	0

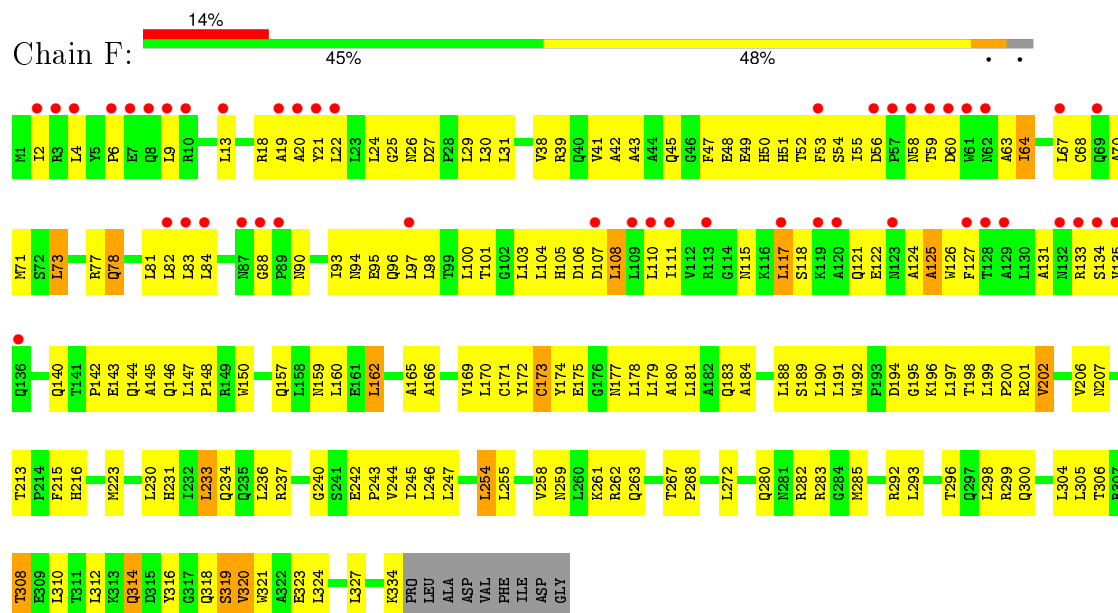
### 3 Residue-property plots

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.

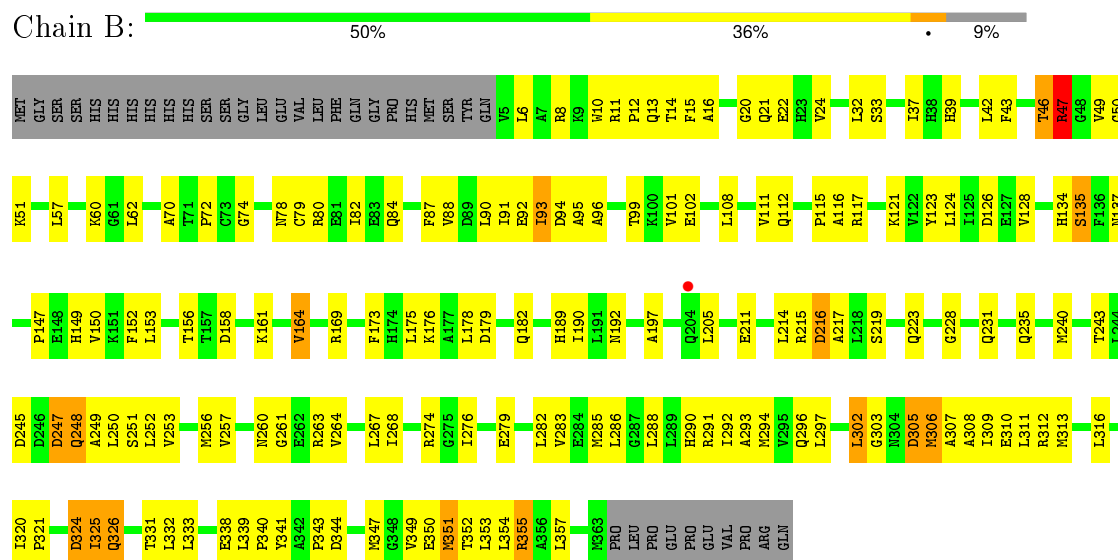
#### • Molecule 1: DNA polymerase III subunit delta

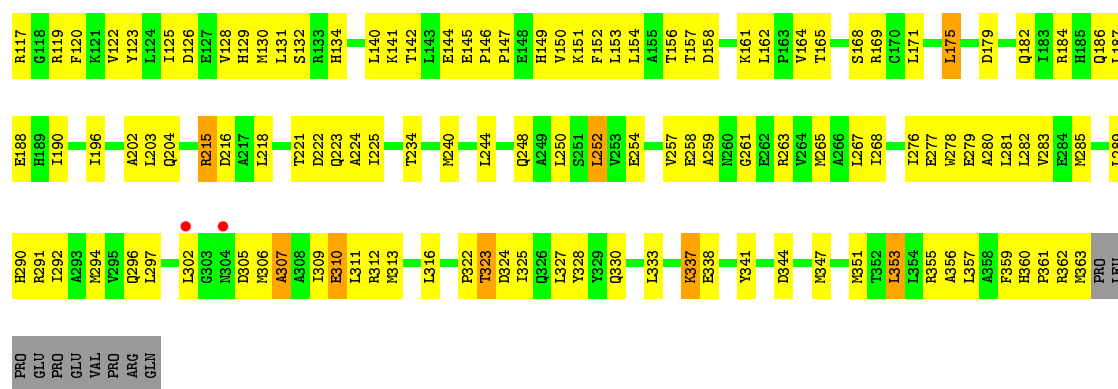


#### • Molecule 1: DNA polymerase III subunit delta

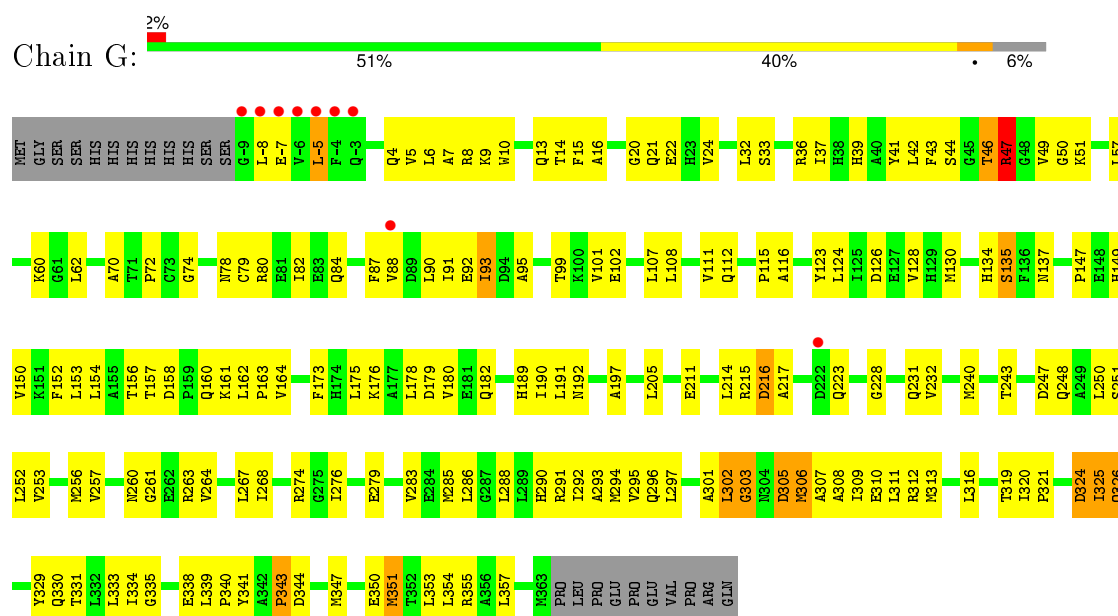


- Molecule 2: DNA polymerase III subunit tau

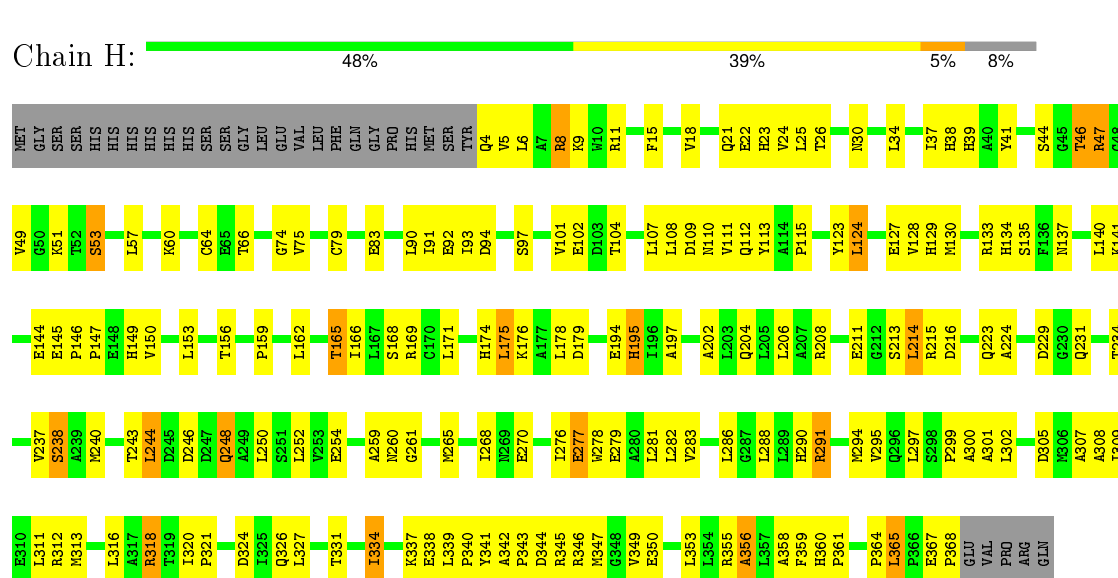




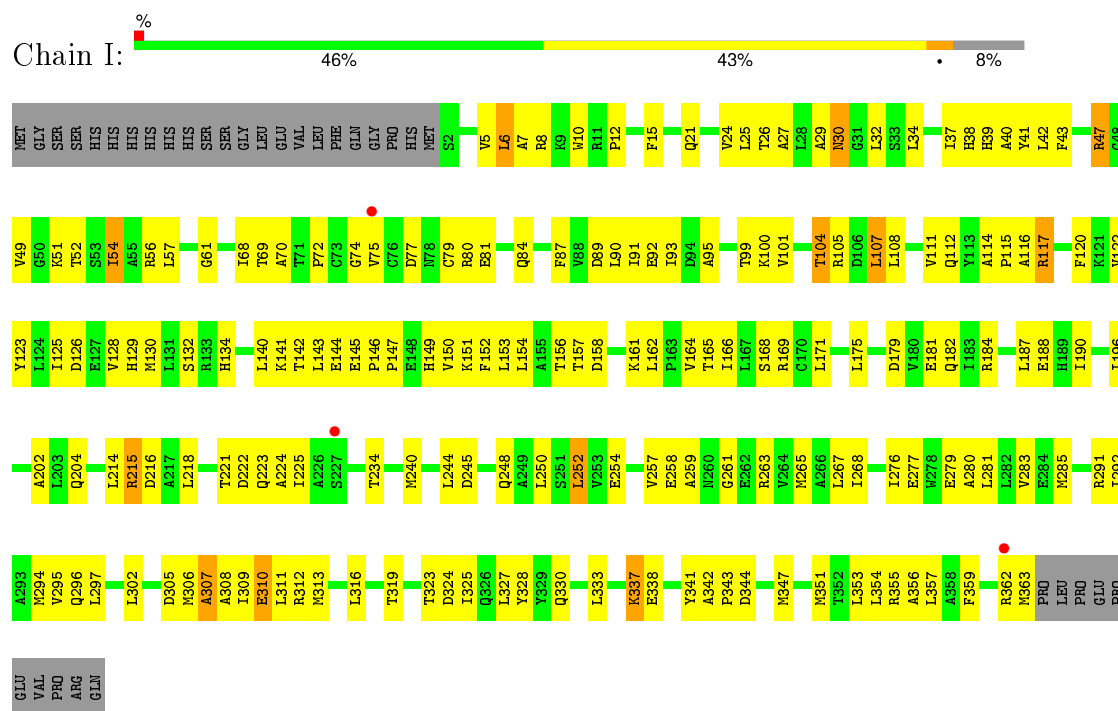
• Molecule 2: DNA polymerase III subunit tau

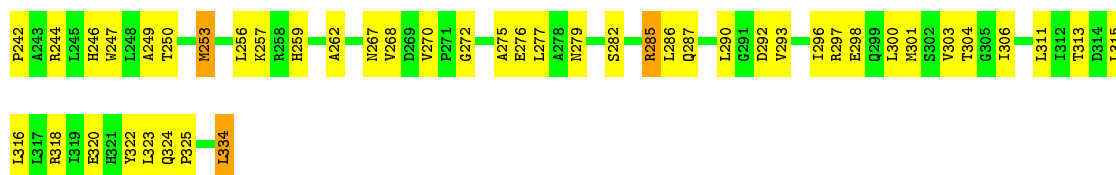


• Molecule 2: DNA polymerase III subunit tau

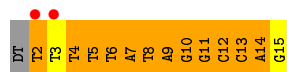


- Molecule 2: DNA polymerase III subunit tau





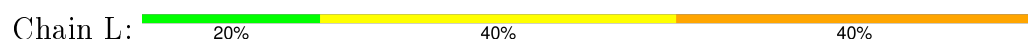
- Molecule 4: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*GP\*GP\*CP\*CP\*AP\*G)-3')



- Molecule 4: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*GP\*GP\*CP\*CP\*AP\*G)-3')



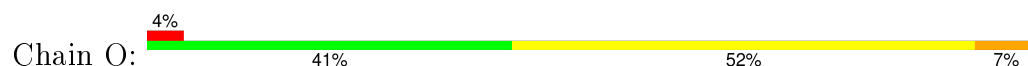
- Molecule 5: DNA (5'-D(\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*AP\*TP\*A)-3')



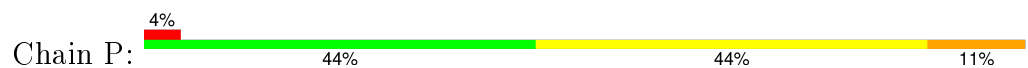
- Molecule 5: DNA (5'-D(\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*AP\*TP\*A)-3')



- Molecule 6: DNA polymerase III subunit psi



- Molecule 6: DNA polymerase III subunit psi





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.69Å 217.18Å 275.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.03 – 3.50 85.42 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (73.03-3.50) 97.5 (85.42-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.222 , 0.257 0.221 , 0.256	Depositor DCC
$R_{free}$ test set	3721 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 73562 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: ZN, BEF, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.53	0/2697	0.66	0/3664
1	F	0.53	0/2706	0.65	1/3675 (0.0%)
2	B	0.57	2/2835 (0.1%)	0.72	0/3841
2	C	0.57	0/2885	0.74	0/3912
2	D	0.58	0/2863	0.78	3/3879 (0.1%)
2	G	0.59	2/2951 (0.1%)	0.75	0/3998
2	H	0.67	2/2885 (0.1%)	0.78	0/3912
2	I	0.67	0/2863	0.82	0/3879
3	E	0.68	0/2666	0.78	1/3639 (0.0%)
3	J	0.66	0/2666	0.77	1/3639 (0.0%)
4	K	1.60	3/320 (0.9%)	2.54	28/492 (5.7%)
4	M	1.65	4/320 (1.2%)	2.53	29/492 (5.9%)
5	L	1.32	1/223 (0.4%)	2.48	22/342 (6.4%)
5	N	1.44	2/223 (0.9%)	2.50	18/342 (5.3%)
6	O	0.60	0/228	0.72	0/307
6	P	0.65	0/228	0.79	0/307
All	All	0.66	16/29559 (0.1%)	0.89	103/40320 (0.3%)

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
2	G	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	127	GLU	CG-CD	6.26	1.61	1.51
4	M	9	DA	C3'-O3'	-6.08	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	326	GLN	CB-CG	5.90	1.68	1.52
4	K	12	DC	C3'-O3'	-5.81	1.36	1.44
5	L	6	DC	C3'-O3'	-5.76	1.36	1.44
2	B	326	GLN	CG-CD	5.58	1.63	1.51
2	H	102	GLU	CG-CD	5.55	1.60	1.51
4	M	7	DA	N9-C4	-5.43	1.34	1.37
4	K	7	DA	N9-C4	-5.34	1.34	1.37
2	G	326	GLN	CB-CG	5.29	1.66	1.52
5	N	5	DC	C3'-O3'	-5.27	1.37	1.44
4	M	10	DG	C3'-O3'	-5.26	1.37	1.44
5	N	6	DC	C3'-O3'	-5.15	1.37	1.44
4	M	12	DC	C3'-O3'	-5.07	1.37	1.44
4	K	13	DC	C3'-O3'	-5.06	1.37	1.44
2	G	326	GLN	CG-CD	5.01	1.62	1.51

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	5	DT	O4'-C1'-N1	-15.54	97.13	108.00
4	K	5	DT	O4'-C1'-N1	-14.21	98.05	108.00
5	L	5	DC	O4'-C4'-C3'	-12.67	98.40	106.00
5	N	5	DC	O4'-C4'-C3'	-12.08	98.75	106.00
5	N	1	DC	O4'-C4'-C3'	-11.92	98.85	106.00
5	N	1	DC	C4'-C3'-C2'	-10.88	93.31	103.10
4	M	14	DA	O4'-C1'-N9	-10.62	100.57	108.00
5	L	1	DC	O4'-C4'-C3'	-10.25	99.85	106.00
4	K	14	DA	O4'-C1'-N9	-10.02	100.99	108.00
5	L	7	DT	N3-C4-O4	9.59	125.65	119.90
4	K	8	DT	C1'-O4'-C4'	-9.22	100.88	110.10
5	L	1	DC	C4'-C3'-C2'	-9.09	94.92	103.10
4	M	8	DT	C1'-O4'-C4'	-9.04	101.06	110.10
5	L	9	DT	C1'-O4'-C4'	-8.86	101.24	110.10
4	K	13	DC	C1'-O4'-C4'	-8.77	101.33	110.10
4	M	7	DA	O4'-C1'-N9	-8.71	101.91	108.00
5	N	7	DT	N3-C4-O4	8.49	124.99	119.90
4	M	13	DC	C1'-O4'-C4'	-8.43	101.67	110.10
4	K	12	DC	O4'-C1'-N1	-8.37	102.14	108.00
4	K	6	DT	O4'-C1'-C2'	-8.23	99.31	105.90
4	K	11	DG	C1'-O4'-C4'	-8.19	101.92	110.10
5	N	9	DT	C1'-O4'-C4'	-8.13	101.97	110.10
4	M	6	DT	C1'-O4'-C4'	-8.07	102.03	110.10
3	J	334	LEU	CA-CB-CG	7.82	133.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	15	DG	O4'-C1'-C2'	-7.74	99.71	105.90
5	L	6	DC	C6-N1-C2	7.72	123.39	120.30
5	N	5	DC	C1'-O4'-C4'	-7.63	102.47	110.10
5	L	7	DT	C5-C4-O4	-7.60	119.58	124.90
5	L	1	DC	C3'-C2'-C1'	-7.40	93.62	102.50
4	K	8	DT	O4'-C4'-C3'	-7.32	101.57	104.50
4	K	15	DG	O4'-C1'-N9	-7.30	102.89	108.00
4	K	9	DA	P-O3'-C3'	-7.29	110.96	119.70
4	K	6	DT	C1'-O4'-C4'	-7.28	102.82	110.10
5	N	2	DT	N3-C4-O4	7.22	124.23	119.90
5	L	1	DC	C6-N1-C2	7.21	123.18	120.30
5	N	1	DC	C3'-C2'-C1'	-7.17	93.90	102.50
4	K	8	DT	P-O5'-C5'	-7.02	109.67	120.90
4	M	8	DT	P-O5'-C5'	-7.00	109.69	120.90
4	M	9	DA	P-O3'-C3'	-6.92	111.39	119.70
5	N	7	DT	C5-C4-O4	-6.91	120.06	124.90
5	N	1	DC	C5-C6-N1	-6.90	117.55	121.00
5	N	1	DC	C6-N1-C2	6.87	123.05	120.30
3	E	334	LEU	CA-CB-CG	6.85	131.06	115.30
5	L	5	DC	C1'-O4'-C4'	-6.79	103.31	110.10
4	M	15	DG	O4'-C1'-N9	-6.79	103.25	108.00
4	M	12	DC	O4'-C1'-N1	-6.74	103.28	108.00
5	L	7	DT	N3-C2-O2	6.63	126.28	122.30
4	M	12	DC	O4'-C1'-C2'	-6.48	100.71	105.90
5	L	2	DT	N3-C4-O4	6.48	123.79	119.90
4	M	9	DA	C2-N3-C4	-6.40	107.40	110.60
5	L	1	DC	C1'-O4'-C4'	-6.35	103.75	110.10
4	K	12	DC	O4'-C1'-C2'	-6.35	100.82	105.90
4	M	11	DG	C2-N3-C4	-6.29	108.75	111.90
4	K	2	DT	P-O3'-C3'	6.26	127.21	119.70
4	M	11	DG	C1'-O4'-C4'	-6.24	103.86	110.10
4	M	10	DG	O4'-C1'-N9	-6.24	103.63	108.00
4	K	4	DT	O4'-C1'-N1	6.02	112.21	108.00
4	K	13	DC	O4'-C4'-C3'	-6.02	102.09	104.50
5	N	2	DT	C5-C4-O4	-6.01	120.69	124.90
5	L	2	DT	C5-C4-O4	-5.94	120.74	124.90
4	M	11	DG	O4'-C4'-C3'	-5.93	102.13	104.50
5	N	7	DT	C1'-O4'-C4'	-5.91	104.19	110.10
5	L	1	DC	C5-C6-N1	-5.91	118.05	121.00
4	K	9	DA	O4'-C1'-N9	-5.85	103.90	108.00
4	M	11	DG	N1-C6-O6	5.77	123.36	119.90
4	M	14	DA	N1-C6-N6	5.76	122.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	8	DT	C5-C4-O4	-5.74	120.88	124.90
5	L	7	DT	N1-C2-O2	-5.74	118.51	123.10
5	N	10	DA	O4'-C1'-C2'	-5.68	101.35	105.90
4	K	9	DA	C2-N3-C4	-5.63	107.79	110.60
4	K	4	DT	C4'-C3'-C2'	-5.59	98.07	103.10
4	M	4	DT	C5-C4-O4	-5.57	121.00	124.90
5	L	4	DG	O4'-C1'-N9	-5.52	104.14	108.00
4	K	4	DT	O4'-C1'-C2'	-5.50	101.50	105.90
4	M	2	DT	P-O3'-C3'	5.49	126.29	119.70
4	M	4	DT	O4'-C1'-C2'	-5.49	101.51	105.90
5	N	4	DG	C5-C6-O6	-5.47	125.32	128.60
5	N	9	DT	O4'-C1'-C2'	-5.46	101.54	105.90
5	L	9	DT	O4'-C1'-C2'	-5.41	101.57	105.90
5	L	10	DA	O4'-C1'-C2'	-5.40	101.58	105.90
4	M	4	DT	C4'-C3'-C2'	-5.35	98.28	103.10
4	K	4	DT	C5-C4-O4	-5.35	121.16	124.90
4	K	10	DG	O4'-C1'-N9	-5.32	104.28	108.00
4	M	15	DG	O4'-C1'-C2'	-5.31	101.65	105.90
4	K	14	DA	N1-C6-N6	5.27	121.76	118.60
1	F	254	LEU	CA-CB-CG	-5.27	103.19	115.30
4	K	7	DA	C4-C5-N7	5.26	113.33	110.70
4	M	13	DC	C6-N1-C2	5.26	122.41	120.30
4	K	12	DC	P-O3'-C3'	-5.18	113.48	119.70
4	M	9	DA	O4'-C1'-N9	-5.18	104.38	108.00
5	N	1	DC	N3-C4-C5	5.16	123.97	121.90
5	L	1	DC	N3-C4-C5	5.13	123.95	121.90
4	M	6	DT	O4'-C1'-C2'	-5.12	101.81	105.90
4	M	10	DG	P-O3'-C3'	-5.09	113.59	119.70
4	K	7	DA	N1-C6-N6	5.09	121.65	118.60
4	M	14	DA	C5-C6-N6	-5.08	119.64	123.70
2	D	175	LEU	CA-CB-CG	5.06	126.93	115.30
5	L	9	DT	C5-C4-O4	-5.05	121.36	124.90
5	L	10	DA	C3'-C2'-C1'	-5.04	96.45	102.50
5	N	10	DA	C8-N9-C4	5.04	107.81	105.80
2	D	360	HIS	C-N-CA	-5.02	100.93	122.00
4	M	11	DG	N3-C4-C5	5.01	131.10	128.60
2	D	353	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	303	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	2703	173	0
1	F	2659	0	2716	181	0
2	B	2791	0	2841	165	1
2	C	2838	0	2886	208	0
2	D	2818	0	2863	205	1
2	G	2903	0	2949	171	1
2	H	2838	0	2886	217	1
2	I	2818	0	2863	212	1
3	E	2601	0	2603	163	1
3	J	2601	0	2603	183	0
4	K	287	0	161	22	0
4	M	287	0	161	22	0
5	L	200	0	115	3	0
5	N	200	0	115	6	0
6	O	224	0	221	26	0
6	P	224	0	221	31	0
7	B	27	0	12	4	0
7	C	27	0	12	4	0
7	D	27	0	12	5	0
7	G	27	0	12	5	0
7	H	27	0	12	4	0
7	I	27	0	12	4	0
8	B	4	0	0	0	0
8	C	4	0	0	0	0
8	D	4	0	0	0	0
8	G	4	0	0	0	0
8	H	4	0	0	0	0
8	I	4	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
All	All	29139	0	28979	1785	3

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 31.

All (1785) 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)
2:I:216:ASP:OD1	3:J:157:SER:HB3	1.35	1.25
2:D:361:PRO:HB2	3:J:272:GLY:HA2	1.23	1.17
2:I:90:LEU:CD1	2:I:122:VAL:HG12	1.86	1.05
3:J:114:VAL:HB	3:J:143:LEU:HD23	1.33	1.05
3:E:114:VAL:HB	3:E:143:LEU:HD23	1.39	1.03
2:B:350:GLU:HB3	2:C:294:MET:HE1	1.39	1.02
2:D:216:ASP:OD1	3:E:157:SER:HB3	1.60	1.01
3:E:2:ARG:HD3	3:E:4:TYR:CE1	1.95	1.00
2:D:90:LEU:CD1	2:D:122:VAL:HG12	1.91	1.00
2:I:90:LEU:HD12	2:I:122:VAL:HG12	1.43	0.98
3:E:3:TRP:HH2	3:E:8:ARG:HG3	1.27	0.98
3:J:114:VAL:HB	3:J:143:LEU:CD2	1.94	0.97
2:B:179:ASP:HB3	2:B:182:GLN:HG3	1.43	0.95
2:D:361:PRO:CB	3:J:272:GLY:HA2	1.96	0.95
3:J:3:TRP:HH2	3:J:8:ARG:HG3	1.29	0.95
2:I:101:VAL:HG23	4:M:10:DG:OP1	1.66	0.95
2:C:244:LEU:HD12	2:C:244:LEU:H	1.32	0.94
2:I:268:ILE:HD11	2:I:353:LEU:HD12	1.46	0.93
2:D:6:LEU:H	2:D:6:LEU:HD12	1.28	0.93
2:G:351:MET:HG2	2:H:290:HIS:HD2	1.31	0.93
4:M:3:DT:H5'	4:M:3:DT:H6	1.34	0.93
3:E:116:ASP:HB3	3:E:119:LEU:HD12	1.47	0.93
2:H:244:LEU:H	2:H:244:LEU:HD12	1.31	0.93
3:J:116:ASP:HB3	3:J:119:LEU:HD12	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:ILE:HD11	2:D:353:LEU:HD12	1.49	0.93
3:J:2:ARG:HD3	3:J:4:TYR:CE1	2.03	0.92
2:B:291:ARG:HG2	2:B:306:MET:HE3	1.48	0.92
2:H:367:GLU:HG3	2:H:368:PRO:HD2	1.49	0.92
2:I:6:LEU:HD12	2:I:6:LEU:H	1.33	0.92
2:D:327:LEU:HD11	6:O:8:GLN:HG2	1.49	0.92
3:E:114:VAL:HB	3:E:143:LEU:CD2	2.00	0.91
2:G:14:THR:HG22	2:G:16:ALA:H	1.35	0.91
2:H:318:ARG:HB2	2:H:318:ARG:NH1	1.86	0.90
1:F:47:PHE:CE1	1:F:77:ARG:HD3	2.07	0.90
2:D:90:LEU:HD12	2:D:122:VAL:HG12	1.50	0.89
1:F:312:LEU:HD13	1:F:320:VAL:HG21	1.53	0.89
2:C:367:GLU:HG3	2:C:368:PRO:HD2	1.52	0.89
4:K:3:DT:H6	4:K:3:DT:H5'	1.34	0.89
2:G:179:ASP:HB3	2:G:182:GLN:HG3	1.55	0.89
1:A:71:MET:SD	1:A:103:LEU:HB3	2.12	0.89
1:A:20:ALA:HB3	1:A:134:SER:HB3	1.52	0.89
2:I:179:ASP:HB3	2:I:182:GLN:HG3	1.54	0.89
2:H:47:ARG:HD2	2:I:164:VAL:HG22	1.52	0.89
3:E:296:ILE:HG13	3:E:315:LEU:HD13	1.54	0.88
1:F:93:ILE:O	1:F:97:LEU:HG	1.73	0.88
1:A:93:ILE:O	1:A:97:LEU:HG	1.73	0.88
2:I:128:VAL:HG12	2:I:156:THR:HB	1.54	0.88
1:A:47:PHE:CE1	1:A:77:ARG:HD3	2.08	0.88
2:H:115:PRO:HD3	2:H:149:HIS:HD2	1.39	0.88
2:D:128:VAL:HG12	2:D:156:THR:HB	1.53	0.88
2:G:351:MET:HG2	2:H:290:HIS:CD2	2.08	0.87
1:F:20:ALA:HB3	1:F:134:SER:HB3	1.56	0.87
2:C:318:ARG:NH1	2:C:318:ARG:HB2	1.89	0.87
2:H:318:ARG:HB2	2:H:318:ARG:HH11	1.38	0.87
1:F:71:MET:SD	1:F:103:LEU:HB3	2.15	0.87
2:G:274:ARG:HH21	2:G:276:ILE:HD11	1.40	0.86
2:B:14:THR:HG22	2:B:16:ALA:H	1.39	0.86
2:G:82:ILE:HG23	2:G:90:LEU:HD23	1.56	0.86
4:M:3:DT:C6	4:M:3:DT:H5'	2.11	0.86
2:H:21:GLN:NE2	2:H:175:LEU:HB3	1.89	0.86
2:D:179:ASP:HB3	2:D:182:GLN:HG3	1.56	0.86
2:C:21:GLN:NE2	2:C:175:LEU:HB3	1.91	0.86
2:H:101:VAL:HG23	4:M:12:DC:OP1	1.76	0.85
2:C:115:PRO:HD3	2:C:149:HIS:HD2	1.40	0.85
1:A:312:LEU:HD13	1:A:320:VAL:HG21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:296:ILE:HG13	3:J:315:LEU:HD13	1.59	0.85
3:E:2:ARG:HD3	3:E:4:TYR:HE1	1.38	0.85
2:G:350:GLU:HB3	2:H:294:MET:HE1	1.57	0.85
2:H:208:ARG:HE	2:H:305:ASP:HB3	1.42	0.85
2:B:351:MET:HG2	2:C:290:HIS:HD2	1.42	0.84
2:H:297:LEU:HA	6:P:25:LEU:HD12	1.58	0.84
2:B:82:ILE:HG23	2:B:90:LEU:HD23	1.59	0.84
1:A:19:ALA:HB1	1:A:104:LEU:HD22	1.60	0.84
2:C:47:ARG:HD2	2:D:164:VAL:HG22	1.59	0.84
4:K:3:DT:C6	4:K:3:DT:H5'	2.12	0.84
1:F:95:GLU:HA	1:F:98:LEU:HD12	1.59	0.84
2:I:90:LEU:CD1	2:I:122:VAL:CG1	2.56	0.83
2:B:302:LEU:HD22	2:B:306:MET:HG3	1.60	0.83
2:I:327:LEU:HD11	6:P:8:GLN:HG2	1.59	0.83
2:G:95:ALA:O	2:G:99:THR:HG22	1.76	0.83
2:G:274:ARG:NH2	2:G:276:ILE:HD11	1.94	0.83
1:F:19:ALA:HB1	1:F:104:LEU:HD22	1.60	0.83
2:G:291:ARG:HG2	2:G:306:MET:CE	2.09	0.83
2:G:291:ARG:HG2	2:G:306:MET:HE3	1.57	0.82
4:M:2:DT:H2"	4:M:3:DT:H5"	1.61	0.82
2:B:95:ALA:O	2:B:99:THR:HG22	1.80	0.82
2:G:-8:LEU:HG	2:G:-8:LEU:O	1.77	0.82
1:A:95:GLU:HA	1:A:98:LEU:HD12	1.60	0.82
2:B:215:ARG:HH11	7:B:400:ADP:H5'1	1.42	0.82
2:G:215:ARG:HH11	7:G:406:ADP:H5'1	1.45	0.81
2:G:21:GLN:OE1	2:G:175:LEU:HB3	1.79	0.81
2:G:302:LEU:HD22	2:G:306:MET:HG3	1.61	0.81
2:I:125:ILE:N	2:I:125:ILE:HD12	1.94	0.81
1:A:49:GLU:HB2	1:A:78:GLN:HB3	1.63	0.81
2:B:51:LYS:HB2	7:B:400:ADP:O2B	1.81	0.81
2:B:291:ARG:HG2	2:B:306:MET:CE	2.11	0.80
2:C:318:ARG:HB2	2:C:318:ARG:HH11	1.45	0.80
3:E:182:MET:HG3	3:E:205:PHE:CE1	2.17	0.80
2:C:208:ARG:HE	2:C:305:ASP:HB3	1.46	0.80
2:D:51:LYS:HB2	7:D:404:ADP:O2B	1.82	0.80
2:I:129:HIS:CD2	2:I:130:MET:HG2	2.17	0.80
1:A:18:ARG:HB3	1:A:133:ARG:O	1.82	0.80
2:I:302:LEU:HD11	2:I:306:MET:HG3	1.62	0.80
2:C:327:LEU:HD23	2:C:361:PRO:HG3	1.64	0.80
3:J:256:LEU:HD11	3:J:287:GLN:HB2	1.63	0.79
2:G:51:LYS:HB2	7:G:406:ADP:O2B	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB1	1:A:199:LEU:HD22	1.65	0.79
1:F:104:LEU:HD13	1:F:133:ARG:HD2	1.64	0.79
2:H:128:VAL:HG12	2:H:156:THR:HB	1.63	0.79
2:G:279:GLU:O	2:G:283:VAL:HG23	1.83	0.79
2:D:362:ARG:O	2:D:363:MET:HG3	1.82	0.79
1:F:39:ARG:NH1	1:F:50:HIS:HB3	1.97	0.79
2:C:268:ILE:HD11	2:C:353:LEU:HD12	1.65	0.79
3:J:224:VAL:HB	3:J:225:PRO:HD3	1.64	0.79
3:E:67:LEU:HD22	3:E:72:THR:O	1.83	0.79
2:G:250:LEU:HD23	2:G:312:ARG:CZ	2.12	0.79
2:G:14:THR:HG22	2:G:16:ALA:N	1.98	0.78
3:E:155:LEU:O	3:E:155:LEU:HD12	1.82	0.78
1:F:267:THR:HB	1:F:268:PRO:HD2	1.64	0.78
4:M:2:DT:H2''	4:M:3:DT:C5'	2.13	0.78
2:I:26:THR:O	2:I:30:ASN:HB2	1.83	0.78
2:B:250:LEU:HD23	2:B:312:ARG:CZ	2.14	0.78
2:B:279:GLU:O	2:B:283:VAL:HG23	1.82	0.78
2:G:101:VAL:HG21	2:G:134:HIS:HB3	1.64	0.78
3:J:155:LEU:O	3:J:155:LEU:HD12	1.83	0.78
1:A:104:LEU:HD13	1:A:133:ARG:HD2	1.66	0.78
1:F:18:ARG:HB3	1:F:133:ARG:O	1.84	0.78
1:A:267:THR:HB	1:A:268:PRO:HD2	1.66	0.77
2:B:14:THR:HG22	2:B:16:ALA:N	1.99	0.77
3:J:121:THR:HG22	3:J:122:ASP:N	1.99	0.77
3:E:285:ARG:CG	3:E:285:ARG:HH11	1.97	0.77
2:D:101:VAL:HG23	4:K:10:DG:OP1	1.85	0.77
2:H:318:ARG:HH11	2:H:318:ARG:CB	1.98	0.77
4:K:2:DT:H2''	4:K:3:DT:H5''	1.64	0.77
1:A:39:ARG:NH1	1:A:50:HIS:HB3	1.98	0.77
2:B:101:VAL:HG21	2:B:134:HIS:HB3	1.66	0.77
2:C:91:ILE:HD12	2:C:123:TYR:CE2	2.19	0.77
1:A:59:THR:HG23	1:A:63:ALA:HB3	1.67	0.77
2:D:90:LEU:CD1	2:D:122:VAL:CG1	2.63	0.76
1:F:49:GLU:HB2	1:F:78:GLN:HB3	1.67	0.76
2:G:252:LEU:HD23	2:G:267:LEU:HD12	1.67	0.76
3:J:3:TRP:CH2	3:J:8:ARG:HG3	2.19	0.76
2:H:47:ARG:HG3	2:I:168:SER:HB2	1.66	0.76
1:F:59:THR:HG23	1:F:63:ALA:HB3	1.68	0.76
3:J:46:ARG:HD2	3:J:68:MET:HG2	1.67	0.76
3:J:182:MET:HG3	3:J:205:PHE:CE1	2.19	0.76
2:D:95:ALA:O	2:D:99:THR:HG22	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:MET:HG2	2:C:290:HIS:CD2	2.19	0.75
3:E:256:LEU:HD11	3:E:287:GLN:HB2	1.66	0.75
2:D:361:PRO:HG2	3:J:275:ALA:HB2	1.68	0.75
1:F:160:LEU:HD11	1:F:189:SER:HB3	1.68	0.75
2:B:21:GLN:OE1	2:B:175:LEU:HB3	1.87	0.75
1:F:98:LEU:HD23	1:F:126:TRP:HB3	1.67	0.75
1:A:104:LEU:HD13	1:A:133:ARG:CD	2.16	0.75
2:I:125:ILE:H	2:I:125:ILE:HD12	1.50	0.75
3:J:285:ARG:HH11	3:J:285:ARG:CG	1.98	0.75
1:A:38:VAL:CG1	1:A:111:ILE:HD11	2.17	0.75
1:F:165:ALA:HB1	1:F:199:LEU:HD22	1.69	0.75
2:C:93:ILE:HD13	2:C:107:LEU:HD13	1.68	0.75
2:G:260:ASN:HD22	2:G:263:ARG:H	1.34	0.75
2:C:21:GLN:NE2	2:C:49:VAL:HG12	2.02	0.75
1:F:104:LEU:HD13	1:F:133:ARG:CD	2.16	0.75
2:C:18:VAL:HB	2:C:25:LEU:HD11	1.67	0.75
2:G:115:PRO:HD3	2:G:149:HIS:HD2	1.51	0.75
2:C:128:VAL:HG12	2:C:156:THR:HB	1.66	0.75
2:D:302:LEU:HD11	2:D:306:MET:HG3	1.67	0.74
1:A:160:LEU:HD11	1:A:189:SER:HB3	1.70	0.74
3:E:3:TRP:CH2	3:E:8:ARG:HG3	2.18	0.74
2:I:215:ARG:HG2	2:I:215:ARG:HH11	1.51	0.74
2:B:350:GLU:HB3	2:C:294:MET:CE	2.17	0.74
2:I:129:HIS:HD1	2:I:156:THR:HG1	1.31	0.74
2:C:259:ALA:HB2	2:C:360:HIS:CE1	2.23	0.74
4:K:2:DT:H2''	4:K:3:DT:C5'	2.17	0.74
1:A:49:GLU:HB3	1:A:51:HIS:CE1	2.22	0.74
2:I:291:ARG:HG2	2:I:291:ARG:HH11	1.53	0.74
1:F:190:LEU:HD21	2:G:36:ARG:HD2	1.69	0.74
2:B:260:ASN:HD22	2:B:263:ARG:H	1.34	0.74
2:I:51:LYS:HB2	7:I:410:ADP:O2B	1.86	0.74
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.68	0.74
2:H:367:GLU:HG3	2:H:368:PRO:CD	2.18	0.74
2:H:327:LEU:HD23	2:H:361:PRO:HG3	1.70	0.74
2:G:74:GLY:HA2	2:G:79:CYS:HB3	1.69	0.74
2:B:42:LEU:HD12	2:B:43:PHE:N	2.02	0.74
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.18	0.74
2:H:259:ALA:HB2	2:H:360:HIS:CE1	2.23	0.73
2:H:268:ILE:HD11	2:H:353:LEU:HD12	1.71	0.73
2:D:26:THR:O	2:D:30:ASN:HB2	1.89	0.73
2:G:216:ASP:OD1	2:H:168:SER:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD11	1:A:183:GLN:HE21	1.54	0.73
1:F:49:GLU:HB3	1:F:51:HIS:CE1	2.23	0.73
2:G:101:VAL:HG21	2:G:134:HIS:CB	2.19	0.73
2:C:331:THR:HA	6:O:14:ILE:HD13	1.70	0.73
2:B:252:LEU:HD23	2:B:267:LEU:HD12	1.71	0.73
2:D:129:HIS:CD2	2:D:130:MET:HG2	2.23	0.73
3:E:224:VAL:HB	3:E:225:PRO:HD3	1.71	0.73
2:H:11:ARG:HG3	2:H:53:SER:HB3	1.71	0.73
2:B:257:VAL:HG11	2:B:320:ILE:HG12	1.70	0.73
3:E:29:ILE:HD13	3:E:40:LEU:HD23	1.70	0.73
2:C:246:ASP:HB3	2:C:309:ILE:HD12	1.71	0.72
2:D:129:HIS:HD1	2:D:156:THR:HG1	1.34	0.72
2:C:318:ARG:HH11	2:C:318:ARG:CB	2.02	0.72
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.19	0.72
2:H:337:LYS:HE2	3:J:334:LEU:HD22	1.71	0.72
2:B:74:GLY:HA2	2:B:79:CYS:HB3	1.71	0.72
1:F:267:THR:OG1	1:F:272:LEU:HD21	1.88	0.72
3:J:41:ILE:HD13	3:J:142:PHE:HB3	1.70	0.72
3:E:121:THR:HG22	3:E:122:ASP:N	2.05	0.72
3:J:30:GLN:HE21	3:J:161:LEU:HD21	1.55	0.72
2:C:101:VAL:HG23	4:K:12:DC:OP1	1.90	0.72
3:J:29:ILE:HD13	3:J:40:LEU:HD23	1.71	0.71
2:B:115:PRO:HD3	2:B:149:HIS:HD2	1.53	0.71
2:H:18:VAL:HB	2:H:25:LEU:HD11	1.71	0.71
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.72	0.71
2:G:354:LEU:HD11	2:H:294:MET:SD	2.30	0.71
2:C:47:ARG:HG3	2:D:168:SER:HB2	1.72	0.71
2:B:101:VAL:HG23	4:K:14:DA:OP1	1.90	0.71
3:J:2:ARG:HD3	3:J:4:TYR:HE1	1.53	0.71
2:C:367:GLU:HG3	2:C:368:PRO:CD	2.20	0.71
3:J:50:CYS:HB3	3:J:53:PRO:HG3	1.72	0.71
2:I:90:LEU:HD13	2:I:122:VAL:CG1	2.19	0.71
2:H:93:ILE:HD13	2:H:107:LEU:HD13	1.71	0.71
1:A:267:THR:OG1	1:A:272:LEU:HD21	1.91	0.71
2:G:108:LEU:O	2:G:111:VAL:HG12	1.90	0.71
2:B:274:ARG:HH21	2:B:276:ILE:HD11	1.55	0.71
2:H:297:LEU:HD23	6:P:25:LEU:CD1	2.20	0.71
2:I:95:ALA:O	2:I:99:THR:HG22	1.91	0.71
1:A:117:LEU:HD12	1:A:122:GLU:HG2	1.73	0.71
2:B:274:ARG:NH2	2:B:276:ILE:HD11	2.06	0.71
2:D:184:ARG:HD3	2:D:204:GLN:NE2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:67:LEU:HD22	3:J:72:THR:O	1.91	0.70
2:D:38:HIS:HD2	2:D:40:ALA:H	1.38	0.70
2:B:268:ILE:HD11	2:B:353:LEU:HD12	1.72	0.70
2:B:179:ASP:HB3	2:B:182:GLN:CG	2.18	0.70
3:E:46:ARG:HD2	3:E:68:MET:HG2	1.70	0.70
2:G:4:GLN:HE21	2:G:9:LYS:HB2	1.57	0.70
1:F:117:LEU:HD12	1:F:122:GLU:HG2	1.73	0.70
2:B:101:VAL:HG21	2:B:134:HIS:CB	2.21	0.70
2:D:125:ILE:HD12	2:D:125:ILE:N	2.07	0.70
1:A:39:ARG:CZ	1:A:50:HIS:HB3	2.22	0.70
1:F:190:LEU:CD2	2:G:36:ARG:HD2	2.21	0.70
1:A:98:LEU:HD23	1:A:126:TRP:HB3	1.74	0.70
2:H:51:LYS:HG2	7:H:408:ADP:O2B	1.92	0.70
1:A:38:VAL:HG11	1:A:111:ILE:HD11	1.72	0.70
2:G:101:VAL:HG23	4:M:14:DA:OP1	1.92	0.70
2:G:161:LYS:HE3	2:H:133:ARG:NH1	2.06	0.70
1:A:162:LEU:HD22	1:A:166:ALA:HB3	1.72	0.70
3:E:50:CYS:HB3	3:E:53:PRO:HG3	1.74	0.70
2:G:49:VAL:HG11	2:G:176:LYS:O	1.91	0.69
2:H:147:PRO:HB2	2:H:149:HIS:CE1	2.27	0.69
2:B:88:VAL:HG11	2:B:116:ALA:HB3	1.74	0.69
2:I:223:GLN:HA	3:J:160:ARG:HD2	1.74	0.69
2:G:80:ARG:O	2:G:84:GLN:HG2	1.92	0.69
2:C:134:HIS:CD2	4:K:12:DC:H4'	2.27	0.69
3:J:285:ARG:HH11	3:J:285:ARG:HG3	1.58	0.69
2:B:197:ALA:HB3	2:B:231:GLN:HG2	1.75	0.69
2:C:144:GLU:HB2	2:C:169:ARG:HE	1.56	0.69
3:E:103:HIS:CD2	3:E:103:HIS:H	2.10	0.69
2:H:341:TYR:HB2	2:I:333:LEU:HD11	1.74	0.69
2:G:257:VAL:HG11	2:G:320:ILE:HG12	1.73	0.69
3:E:41:ILE:HD13	3:E:142:PHE:HB3	1.74	0.69
1:A:28:PRO:HB3	2:B:164:VAL:HG21	1.75	0.69
2:I:184:ARG:HD3	2:I:204:GLN:NE2	2.07	0.69
2:H:91:ILE:HD12	2:H:123:TYR:CE2	2.28	0.69
1:F:38:VAL:CG1	1:F:111:ILE:HD11	2.23	0.69
2:C:147:PRO:HB2	2:C:149:HIS:CE1	2.28	0.69
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.75	0.68
1:A:282:ARG:HD3	1:A:285:MET:HE2	1.75	0.68
2:H:299:PRO:HD3	6:P:28:GLU:HA	1.76	0.68
2:D:38:HIS:HB3	2:D:41:TYR:CE1	2.28	0.68
2:D:215:ARG:HG2	3:E:157:SER:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:HD13	2:D:122:VAL:CG1	2.23	0.68
2:C:101:VAL:CG2	2:C:134:HIS:HB3	2.24	0.68
1:F:162:LEU:HD22	1:F:166:ALA:HB3	1.75	0.68
2:H:144:GLU:HB2	2:H:169:ARG:HE	1.57	0.68
2:H:21:GLN:NE2	2:H:49:VAL:HG12	2.08	0.68
2:H:208:ARG:NE	2:H:305:ASP:HB3	2.07	0.68
3:E:30:GLN:HE21	3:E:161:LEU:HD21	1.59	0.68
2:H:101:VAL:CG2	2:H:134:HIS:HB3	2.23	0.68
3:E:88:LEU:HD23	3:E:120:LEU:HD23	1.75	0.68
1:F:304:LEU:HD23	1:F:327:LEU:HD13	1.76	0.68
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.24	0.68
2:C:129:HIS:ND1	2:C:156:THR:OG1	2.24	0.68
2:I:93:ILE:HD11	2:I:107:LEU:HD21	1.75	0.68
2:I:21:GLN:NE2	2:I:49:VAL:HG13	2.09	0.67
2:B:49:VAL:HG11	2:B:176:LYS:O	1.93	0.67
2:C:11:ARG:HG3	2:C:53:SER:HB3	1.75	0.67
2:D:215:ARG:HG2	2:D:215:ARG:HH11	1.58	0.67
2:I:302:LEU:CD1	2:I:306:MET:HG3	2.24	0.67
2:B:80:ARG:O	2:B:84:GLN:HG2	1.93	0.67
2:C:112:GLN:NE2	2:C:113:TYR:HE1	1.93	0.67
2:I:38:HIS:HD2	2:I:40:ALA:H	1.39	0.67
2:G:152:PHE:O	2:G:153:LEU:HD23	1.95	0.67
2:I:291:ARG:HG2	2:I:291:ARG:NH1	2.09	0.67
1:F:179:LEU:HD11	1:F:183:GLN:HE21	1.58	0.67
2:B:343:PRO:HG3	2:C:286:LEU:HB3	1.75	0.67
2:H:278:TRP:NE1	2:H:346:ARG:HB2	2.10	0.67
2:D:90:LEU:HD12	2:D:122:VAL:O	1.94	0.67
2:H:46:THR:O	2:H:49:VAL:HG23	1.94	0.67
2:C:339:LEU:N	2:C:340:PRO:HD2	2.09	0.67
1:F:304:LEU:O	1:F:308:THR:HG23	1.94	0.67
2:D:21:GLN:NE2	2:D:49:VAL:HG13	2.10	0.67
2:H:11:ARG:CG	2:H:53:SER:HB3	2.24	0.66
1:F:52:THR:HG22	1:F:81:LEU:HD23	1.77	0.66
3:J:103:HIS:H	3:J:103:HIS:CD2	2.11	0.66
2:H:112:GLN:NE2	2:H:113:TYR:HE1	1.92	0.66
2:D:265:MET:HE2	3:E:257:LYS:HD3	1.76	0.66
2:B:331:THR:HG23	6:O:17:TRP:CH2	2.31	0.66
2:G:197:ALA:HB3	2:G:231:GLN:HG2	1.78	0.66
2:G:47:ARG:O	2:G:47:ARG:HG2	1.95	0.66
2:B:47:ARG:HD3	2:B:47:ARG:N	2.09	0.66
2:D:291:ARG:HH11	2:D:291:ARG:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:LEU:O	2:B:111:VAL:HG12	1.95	0.66
2:I:24:VAL:HG21	2:I:175:LEU:HD22	1.78	0.66
1:A:49:GLU:HB3	1:A:51:HIS:HE1	1.58	0.66
2:C:101:VAL:HG22	2:C:134:HIS:HB3	1.77	0.66
2:I:362:ARG:O	2:I:363:MET:HG3	1.95	0.66
2:B:147:PRO:HB2	2:B:150:VAL:HG23	1.78	0.65
2:G:39:HIS:CD2	2:G:39:HIS:H	2.12	0.65
4:M:8:DT:H2''	4:M:9:DA:O5'	1.95	0.65
1:F:49:GLU:HB3	1:F:51:HIS:HE1	1.61	0.65
2:C:208:ARG:NE	2:C:305:ASP:HB3	2.11	0.65
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.77	0.65
2:I:93:ILE:HD11	2:I:107:LEU:CD2	2.26	0.65
3:J:169:GLU:O	3:J:173:VAL:HG23	1.96	0.65
1:F:101:THR:HG21	1:F:126:TRP:HB2	1.77	0.65
2:I:38:HIS:HB3	2:I:41:TYR:CE1	2.31	0.65
2:I:351:MET:HG2	3:J:253:MET:HE1	1.77	0.65
2:D:361:PRO:HG2	3:J:275:ALA:CB	2.25	0.65
1:F:64:ILE:HG12	1:F:64:ILE:O	1.97	0.65
2:H:246:ASP:HB3	2:H:309:ILE:HD12	1.78	0.65
2:I:150:VAL:O	2:I:151:LYS:HD3	1.96	0.65
1:A:71:MET:HB2	1:A:108:LEU:HG	1.78	0.65
2:B:47:ARG:HG2	2:B:47:ARG:O	1.95	0.65
2:G:350:GLU:HB3	2:H:294:MET:CE	2.27	0.65
2:I:309:ILE:O	2:I:311:LEU:N	2.29	0.65
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.78	0.65
3:J:32:LEU:O	3:J:35:MET:HB2	1.97	0.65
2:G:115:PRO:HD3	2:G:149:HIS:CD2	2.31	0.65
2:D:302:LEU:CD1	2:D:306:MET:HG3	2.26	0.65
2:H:101:VAL:CG2	4:M:12:DC:H5''	2.27	0.64
2:G:32:LEU:HA	2:G:37:ILE:HD11	1.78	0.64
3:J:285:ARG:NH1	3:J:285:ARG:HG3	2.11	0.64
2:I:74:GLY:HA2	2:I:79:CYS:HB3	1.79	0.64
1:F:334:LYS:C	1:F:334:LYS:HD3	2.18	0.64
2:H:129:HIS:ND1	2:H:156:THR:OG1	2.28	0.64
3:E:285:ARG:NH1	3:E:285:ARG:HG3	2.12	0.64
3:E:106:LEU:HD23	3:E:106:LEU:O	1.97	0.64
2:B:39:HIS:CD2	2:B:39:HIS:H	2.16	0.64
2:H:64:CYS:SG	2:H:66:THR:HG23	2.37	0.64
2:D:327:LEU:HD11	6:O:8:GLN:CG	2.25	0.64
2:D:77:ASP:O	2:D:81:GLU:HG3	1.98	0.64
2:G:179:ASP:HB3	2:G:182:GLN:CG	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:VAL:HG21	2:G:175:LEU:CD2	2.28	0.64
2:D:263:ARG:O	2:D:267:LEU:HB2	1.98	0.64
2:D:74:GLY:HA2	2:D:79:CYS:HB3	1.80	0.64
3:E:20:ALA:CB	3:E:22:ARG:HG3	2.28	0.64
2:D:129:HIS:ND1	2:D:156:THR:OG1	2.24	0.63
2:G:252:LEU:HD21	2:G:267:LEU:HB2	1.78	0.63
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.80	0.63
2:G:42:LEU:HD12	2:G:43:PHE:N	2.12	0.63
2:D:309:ILE:O	2:D:311:LEU:N	2.32	0.63
2:C:104:THR:OG1	2:C:135:SER:HB2	1.99	0.63
2:B:252:LEU:HD21	2:B:267:LEU:HB2	1.80	0.63
2:B:32:LEU:HA	2:B:37:ILE:HD11	1.81	0.63
2:I:90:LEU:HD12	2:I:122:VAL:O	1.99	0.63
2:C:337:LYS:HE2	3:E:334:LEU:HD22	1.81	0.63
2:G:290:HIS:O	2:G:294:MET:HG3	1.97	0.63
2:H:104:THR:OG1	2:H:135:SER:HB2	1.98	0.63
3:J:253:MET:HE2	3:J:290:LEU:HD21	1.81	0.63
1:A:48:GLU:O	1:A:50:HIS:CD2	2.52	0.62
3:E:285:ARG:HH11	3:E:285:ARG:HG3	1.63	0.62
2:H:324:ASP:O	2:H:327:LEU:HB3	1.98	0.62
2:B:115:PRO:HD3	2:B:149:HIS:CD2	2.32	0.62
2:I:362:ARG:HD3	6:P:4:ARG:HG2	1.79	0.62
1:F:282:ARG:HD3	1:F:285:MET:HE2	1.80	0.62
2:I:362:ARG:HG2	6:P:4:ARG:CZ	2.28	0.62
2:H:101:VAL:HG22	2:H:134:HIS:HB3	1.80	0.62
3:E:169:GLU:O	3:E:173:VAL:HG23	1.98	0.62
2:I:77:ASP:O	2:I:81:GLU:HG3	2.00	0.62
2:I:265:MET:HE2	3:J:257:LYS:HD3	1.80	0.62
2:B:354:LEU:HD11	2:C:294:MET:SD	2.39	0.62
1:A:101:THR:HG21	1:A:126:TRP:HB2	1.79	0.62
2:I:70:ALA:O	2:I:72:PRO:HD3	1.99	0.62
1:F:71:MET:HB2	1:F:108:LEU:HG	1.81	0.62
2:I:70:ALA:C	2:I:72:PRO:HD3	2.19	0.62
1:A:282:ARG:HD3	1:A:285:MET:CE	2.29	0.62
3:J:106:LEU:O	3:J:106:LEU:HD23	2.00	0.62
2:B:24:VAL:HG21	2:B:175:LEU:CD2	2.29	0.62
2:G:47:ARG:N	2:G:47:ARG:HD3	2.15	0.62
2:C:278:TRP:NE1	2:C:346:ARG:HB2	2.14	0.62
1:F:77:ARG:HG2	1:F:107:ASP:HA	1.81	0.62
2:C:21:GLN:HE21	2:C:49:VAL:HG12	1.65	0.62
2:D:252:LEU:HD13	2:D:285:MET:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:GLU:O	2:D:280:ALA:HB3	2.00	0.61
1:A:48:GLU:O	1:A:50:HIS:HD2	1.82	0.61
2:H:115:PRO:HD3	2:H:149:HIS:CD2	2.28	0.61
3:E:279:ASN:O	3:J:282:SER:HB2	1.99	0.61
2:C:297:LEU:HA	6:O:25:LEU:HD12	1.81	0.61
2:D:6:LEU:H	2:D:6:LEU:CD1	2.10	0.61
3:J:121:THR:HG22	3:J:122:ASP:H	1.63	0.61
2:H:337:LYS:CE	3:J:334:LEU:HD22	2.31	0.61
2:D:32:LEU:HD23	2:D:37:ILE:CD1	2.30	0.61
1:F:237:ARG:HG3	1:F:321:TRP:CE2	2.36	0.61
2:B:290:HIS:O	2:B:294:MET:HG3	2.00	0.61
3:E:11:PHE:CZ	3:E:15:VAL:HG21	2.34	0.61
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.35	0.61
1:F:48:GLU:HG3	1:F:49:GLU:H	1.65	0.61
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.83	0.61
2:I:215:ARG:HG2	3:J:157:SER:HB2	1.82	0.61
2:C:297:LEU:HD23	6:O:25:LEU:CD1	2.31	0.61
2:H:297:LEU:HD23	6:P:25:LEU:HD13	1.81	0.61
2:C:46:THR:O	2:C:49:VAL:HG23	2.00	0.61
1:F:160:LEU:HD22	1:F:195:GLY:HA2	1.83	0.61
2:D:87:PHE:CE2	2:D:89:ASP:HB2	2.36	0.61
3:J:20:ALA:CB	3:J:22:ARG:HG3	2.31	0.61
2:H:24:VAL:HG21	2:H:175:LEU:HD22	1.83	0.61
3:J:46:ARG:CD	3:J:68:MET:HG2	2.31	0.61
2:D:38:HIS:CD2	2:D:40:ALA:H	2.19	0.61
1:F:38:VAL:HG11	1:F:111:ILE:HD11	1.83	0.61
3:J:213:ARG:HG2	3:J:213:ARG:HH11	1.66	0.61
2:H:47:ARG:HD2	2:I:164:VAL:CG2	2.26	0.61
2:I:7:ALA:O	7:I:410:ADP:O3'	2.19	0.61
2:D:125:ILE:HD12	2:D:125:ILE:H	1.65	0.61
2:D:291:ARG:NH1	2:D:291:ARG:HG2	2.14	0.61
2:D:252:LEU:HD13	2:D:285:MET:HE1	1.83	0.61
2:I:257:VAL:HG12	2:I:328:TYR:CE2	2.36	0.61
4:K:8:DT:H2''	4:K:9:DA:O5'	2.01	0.60
1:F:169:VAL:HG21	1:F:199:LEU:HD11	1.83	0.60
3:J:88:LEU:HD23	3:J:120:LEU:HD23	1.83	0.60
1:F:48:GLU:O	1:F:50:HIS:CD2	2.54	0.60
2:H:101:VAL:HG23	4:M:12:DC:H5''	1.82	0.60
2:B:260:ASN:ND2	2:B:263:ARG:H	1.98	0.60
2:I:263:ARG:O	2:I:267:LEU:HB2	2.01	0.60
2:I:69:THR:HG21	2:I:72:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:TYR:CE2	2:H:171:LEU:HD12	2.37	0.60
2:C:21:GLN:HE22	2:C:175:LEU:HB3	1.67	0.60
2:C:295:VAL:HG22	2:C:302:LEU:HB2	1.83	0.60
2:H:297:LEU:HD22	6:P:25:LEU:HA	1.83	0.60
2:C:324:ASP:O	2:C:327:LEU:HB3	2.02	0.60
2:H:51:LYS:CG	7:H:408:ADP:O2B	2.50	0.60
2:H:339:LEU:N	2:H:340:PRO:HD2	2.17	0.60
1:A:169:VAL:HG21	1:A:199:LEU:HD11	1.84	0.60
2:I:21:GLN:NE2	2:I:49:VAL:CG1	2.64	0.60
3:J:34:GLY:HA3	3:J:200:ALA:HB2	1.82	0.60
2:H:299:PRO:HG2	6:P:28:GLU:HG2	1.84	0.60
1:A:71:MET:CB	1:A:108:LEU:HG	2.32	0.60
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.83	0.60
1:A:64:ILE:O	1:A:64:ILE:HG12	2.01	0.60
2:I:147:PRO:HD2	2:I:150:VAL:HB	1.82	0.59
2:D:24:VAL:HG21	2:D:175:LEU:HD22	1.84	0.59
2:I:8:ARG:NH1	3:J:135:PRO:HD2	2.17	0.59
2:C:367:GLU:CG	2:C:368:PRO:HD2	2.27	0.59
2:C:115:PRO:HD3	2:C:149:HIS:CD2	2.30	0.59
2:I:30:ASN:O	2:I:34:LEU:HG	2.02	0.59
2:C:51:LYS:HG2	7:C:402:ADP:O2B	2.01	0.59
1:A:304:LEU:O	1:A:308:THR:HG23	2.01	0.59
1:A:160:LEU:HD22	1:A:195:GLY:HA2	1.82	0.59
2:I:223:GLN:HG2	2:I:240:MET:SD	2.43	0.59
2:B:152:PHE:O	2:B:153:LEU:HD23	2.02	0.59
2:B:256:MET:HA	2:B:357:LEU:HD21	1.85	0.59
1:F:306:THR:HG23	3:J:311:LEU:HD12	1.85	0.59
2:D:261:GLY:HA3	3:E:260:HIS:ND1	2.17	0.59
2:I:122:VAL:HG22	2:I:151:LYS:HB2	1.85	0.59
2:H:243:THR:HG22	2:H:244:LEU:O	2.02	0.59
2:C:290:HIS:NE2	2:C:294:MET:HE1	2.17	0.59
3:J:29:ILE:CD1	3:J:40:LEU:HD23	2.33	0.59
1:A:24:LEU:HD11	1:A:117:LEU:HD11	1.85	0.59
2:D:30:ASN:O	2:D:34:LEU:HG	2.03	0.59
2:C:101:VAL:HA	2:C:135:SER:HB3	1.84	0.59
2:C:340:PRO:HB2	2:C:341:TYR:CD1	2.36	0.59
2:D:70:ALA:C	2:D:72:PRO:HD3	2.22	0.59
3:E:298:GLU:HA	3:E:298:GLU:OE1	2.02	0.59
2:G:331:THR:HG23	6:P:17:TRP:CH2	2.37	0.59
2:H:297:LEU:HD23	6:P:25:LEU:HD12	1.85	0.59
1:A:77:ARG:HG2	1:A:107:ASP:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:VAL:HG13	2:C:150:VAL:HG21	1.83	0.59
2:G:24:VAL:HG22	2:G:173:PHE:HB3	1.85	0.59
2:H:321:PRO:O	2:H:324:ASP:HB2	2.03	0.59
3:J:72:THR:O	3:J:72:THR:HG23	2.03	0.59
3:J:99:LYS:CE	3:J:105:ARG:HH22	2.16	0.59
3:E:76:TYR:HD1	3:E:111:VAL:CG2	2.16	0.59
3:J:114:VAL:CB	3:J:143:LEU:CD2	2.77	0.59
2:H:290:HIS:NE2	2:H:294:MET:HE1	2.17	0.59
2:C:47:ARG:HD2	2:D:164:VAL:CG2	2.33	0.59
2:D:21:GLN:NE2	2:D:49:VAL:CG1	2.66	0.59
2:B:355:ARG:NH2	2:C:330:GLN:OE1	2.36	0.59
1:F:198:THR:OG1	1:F:200:PRO:HG2	2.03	0.59
2:C:321:PRO:O	2:C:324:ASP:HB2	2.02	0.58
2:D:363:MET:SD	3:J:276:GLU:OE1	2.61	0.58
1:F:24:LEU:HD22	1:F:115:ASN:O	2.03	0.58
3:E:259:HIS:CE1	3:J:259:HIS:CE1	2.91	0.58
2:D:7:ALA:O	7:D:404:ADP:O3'	2.19	0.58
2:I:6:LEU:CD1	2:I:6:LEU:H	2.13	0.58
1:A:48:GLU:HG3	1:A:49:GLU:H	1.68	0.58
2:G:88:VAL:HG11	2:G:116:ALA:HB3	1.85	0.58
2:H:299:PRO:CG	6:P:28:GLU:HG2	2.33	0.58
1:A:52:THR:HG22	1:A:81:LEU:HD23	1.83	0.58
1:F:48:GLU:O	1:F:50:HIS:HD2	1.86	0.58
1:F:71:MET:CB	1:F:108:LEU:HG	2.33	0.58
2:D:70:ALA:O	2:D:72:PRO:HD3	2.03	0.58
2:I:277:GLU:O	2:I:280:ALA:HB3	2.03	0.58
2:C:175:LEU:HD23	2:C:175:LEU:N	2.18	0.58
2:I:80:ARG:O	2:I:84:GLN:HG3	2.03	0.58
2:H:15:PHE:CE1	2:H:57:LEU:HB3	2.39	0.58
2:H:101:VAL:HA	2:H:135:SER:HB3	1.85	0.58
3:E:28:LEU:O	3:E:161:LEU:HD12	2.03	0.58
2:I:362:ARG:HG2	6:P:4:ARG:NE	2.18	0.58
2:I:252:LEU:HD13	2:I:285:MET:CE	2.34	0.58
3:E:29:ILE:CD1	3:E:40:LEU:HD23	2.33	0.58
1:A:304:LEU:HD23	1:A:327:LEU:HD13	1.85	0.58
3:E:32:LEU:O	3:E:35:MET:HB2	2.03	0.58
2:H:282:LEU:O	2:H:286:LEU:HD12	2.02	0.58
2:D:309:ILE:HG21	2:D:313:MET:HG2	1.85	0.58
2:C:137:ASN:H	2:C:137:ASN:HD22	1.51	0.58
1:F:319:SER:O	1:F:321:TRP:N	2.36	0.58
2:D:80:ARG:O	2:D:84:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:178:LEU:HD12	2:G:214:LEU:HB2	1.85	0.58
3:J:11:PHE:CZ	3:J:15:VAL:HG21	2.39	0.58
2:I:268:ILE:HD11	2:I:353:LEU:CD1	2.27	0.58
2:I:125:ILE:H	2:I:125:ILE:CD1	2.15	0.58
3:E:72:THR:O	3:E:72:THR:HG23	2.04	0.58
2:D:26:THR:HG22	2:D:27:ALA:N	2.18	0.58
3:E:172:ALA:HB1	3:E:191:LEU:HD11	1.85	0.58
2:D:362:ARG:HD3	6:O:4:ARG:HG2	1.86	0.58
2:I:90:LEU:HD13	2:I:122:VAL:HG11	1.84	0.57
3:E:259:HIS:ND1	3:J:259:HIS:CE1	2.71	0.57
1:F:21:TYR:CE1	1:F:135:VAL:HB	2.39	0.57
2:G:256:MET:HA	2:G:357:LEU:HD21	1.86	0.57
2:D:150:VAL:O	2:D:151:LYS:HD3	2.03	0.57
2:I:125:ILE:N	2:I:125:ILE:CD1	2.65	0.57
2:C:11:ARG:CG	2:C:53:SER:HB3	2.34	0.57
2:I:87:PHE:CE2	2:I:89:ASP:HB2	2.39	0.57
2:D:122:VAL:HG22	2:D:151:LYS:HB2	1.86	0.57
2:C:244:LEU:CD1	2:C:244:LEU:H	2.12	0.57
1:A:97:LEU:HD13	1:A:126:TRP:CH2	2.39	0.57
2:I:323:THR:HG21	6:P:8:GLN:OE1	2.03	0.57
4:K:12:DC:H2''	4:K:13:DC:O5'	2.03	0.57
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.35	0.57
2:C:51:LYS:CG	7:C:402:ADP:O2B	2.52	0.57
3:J:76:TYR:HD1	3:J:111:VAL:CG2	2.17	0.57
3:E:99:LYS:CE	3:E:105:ARG:HH22	2.17	0.57
2:D:114:ALA:HB1	2:D:115:PRO:HD2	1.86	0.57
1:A:56:ASP:HB2	1:A:58:ASN:HB2	1.87	0.57
2:B:20:GLY:O	2:B:21:GLN:HB2	2.05	0.57
3:J:285:ARG:NH1	3:J:285:ARG:CG	2.63	0.57
2:I:309:ILE:HG21	2:I:313:MET:HG2	1.85	0.57
1:A:26:ASN:ND2	1:A:140:GLN:OE1	2.36	0.57
2:C:41:TYR:CE2	2:C:171:LEU:HD12	2.39	0.57
1:F:59:THR:HG23	1:F:63:ALA:CB	2.35	0.57
2:C:338:GLU:OE2	2:C:355:ARG:NH2	2.37	0.57
2:D:10:TRP:CE2	2:D:190:ILE:HG23	2.39	0.57
1:F:56:ASP:HB2	1:F:58:ASN:HB2	1.87	0.57
2:C:337:LYS:CE	3:E:334:LEU:HD22	2.35	0.57
3:J:199:GLY:HA2	3:J:202:LEU:HB2	1.87	0.57
2:D:93:ILE:HD11	2:D:107:LEU:CD2	2.35	0.57
2:H:331:THR:HA	6:P:14:ILE:HD13	1.87	0.57
1:F:244:VAL:HG21	4:M:5:DT:H71	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:129:HIS:ND1	2:I:156:THR:OG1	2.27	0.57
3:J:222:TYR:O	3:J:225:PRO:HD2	2.05	0.57
2:B:261:GLY:HA3	2:C:297:LEU:HD11	1.87	0.56
3:J:213:ARG:HH21	3:J:267:ASN:HD22	1.52	0.56
1:F:21:TYR:CD1	1:F:135:VAL:HB	2.40	0.56
2:I:32:LEU:HD23	2:I:37:ILE:CD1	2.34	0.56
2:G:147:PRO:HB2	2:G:150:VAL:HG23	1.86	0.56
3:J:298:GLU:HA	3:J:298:GLU:OE1	2.05	0.56
2:I:47:ARG:HG2	2:I:47:ARG:O	2.06	0.56
3:E:86:ASN:O	3:E:119:LEU:HD22	2.05	0.56
2:H:21:GLN:HE21	2:H:49:VAL:HG12	1.68	0.56
2:C:115:PRO:CD	2:C:149:HIS:HD2	2.16	0.56
3:E:52:GLN:N	3:E:53:PRO:HD3	2.21	0.56
2:H:234:THR:O	2:H:238:SER:OG	2.22	0.56
2:B:214:LEU:O	2:B:217:ALA:HB3	2.05	0.56
2:G:347:MET:CE	2:H:291:ARG:HH21	2.19	0.56
2:H:22:GLU:O	2:H:26:THR:HB	2.06	0.56
2:C:290:HIS:CE1	2:C:294:MET:HE2	2.40	0.56
2:H:134:HIS:CD2	4:M:12:DC:H4'	2.40	0.56
2:I:38:HIS:CD2	2:I:40:ALA:H	2.21	0.56
2:I:114:ALA:HB1	2:I:115:PRO:HD2	1.87	0.56
3:E:118:ALA:HB2	3:E:145:THR:HG22	1.87	0.56
2:D:147:PRO:HD2	2:D:150:VAL:HB	1.87	0.56
1:F:198:THR:HG23	1:F:201:ARG:HD2	1.88	0.56
2:B:8:ARG:NH1	2:C:146:PRO:HD2	2.21	0.56
3:E:285:ARG:CG	3:E:285:ARG:NH1	2.61	0.56
2:D:5:VAL:HG13	2:D:222:ASP:OD2	2.06	0.56
3:J:118:ALA:HB2	3:J:145:THR:HG22	1.87	0.56
2:C:128:VAL:HG22	2:C:128:VAL:O	2.06	0.56
2:B:292:ILE:CD1	2:B:316:LEU:HD23	2.36	0.56
3:J:172:ALA:HB1	3:J:191:LEU:HD11	1.87	0.56
3:J:46:ARG:NH1	3:J:69:GLN:HG3	2.21	0.56
2:D:254:GLU:OE2	2:D:312:ARG:HD2	2.05	0.56
2:H:113:TYR:N	2:H:113:TYR:CD1	2.73	0.56
3:E:99:LYS:HD3	3:E:105:ARG:NH2	2.21	0.56
2:G:128:VAL:O	2:G:128:VAL:HG22	2.06	0.56
1:A:188:LEU:HD13	1:A:197:LEU:HD13	1.87	0.56
1:F:98:LEU:CD2	1:F:126:TRP:HB3	2.36	0.56
1:A:24:LEU:HD22	1:A:115:ASN:O	2.05	0.56
2:D:265:MET:CE	3:E:257:LYS:HD3	2.35	0.56
2:H:214:LEU:O	2:H:214:LEU:HD12	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ASN:O	1:F:263:GLN:HG3	2.06	0.56
6:P:26:GLN:O	6:P:28:GLU:N	2.38	0.55
2:H:21:GLN:HE22	2:H:175:LEU:HB3	1.66	0.55
2:H:137:ASN:HA	2:H:140:LEU:HG	1.86	0.55
1:F:199:LEU:N	1:F:200:PRO:HD2	2.21	0.55
2:I:254:GLU:OE1	2:I:312:ARG:NH1	2.38	0.55
2:G:338:GLU:C	2:G:340:PRO:HD2	2.25	0.55
2:D:100:LYS:O	2:D:104:THR:HG23	2.06	0.55
2:D:323:THR:HG21	6:O:8:GLN:OE1	2.06	0.55
3:E:292:ASP:HB3	3:E:315:LEU:CD1	2.35	0.55
1:A:198:THR:OG1	1:A:200:PRO:HG2	2.06	0.55
3:J:46:ARG:HH12	3:J:69:GLN:HG3	1.72	0.55
2:G:260:ASN:ND2	2:G:263:ARG:H	2.04	0.55
3:E:207:GLY:C	3:E:209:ASN:H	2.09	0.55
1:F:318:GLN:H	1:F:318:GLN:CD	2.09	0.55
1:A:59:THR:HG23	1:A:63:ALA:CB	2.35	0.55
3:J:81:PRO:HB3	3:J:87:THR:O	2.06	0.55
2:D:223:GLN:HG2	2:D:240:MET:SD	2.47	0.55
1:F:213:THR:H	1:F:216:HIS:CD2	2.25	0.55
3:J:82:GLU:HA	3:J:82:GLU:OE1	2.06	0.55
6:O:9:LEU:HD12	6:O:16:GLN:NE2	2.22	0.55
1:F:296:THR:O	1:F:300:GLN:HG3	2.07	0.55
2:D:351:MET:HG2	3:E:253:MET:HE1	1.88	0.55
1:A:199:LEU:N	1:A:200:PRO:HD2	2.22	0.55
3:J:121:THR:CG2	3:J:122:ASP:N	2.68	0.55
3:J:213:ARG:HG2	3:J:213:ARG:NH1	2.21	0.55
3:J:99:LYS:HD3	3:J:105:ARG:NH2	2.21	0.55
2:D:15:PHE:CE2	2:D:57:LEU:HB3	2.42	0.55
2:B:309:ILE:HG22	2:B:313:MET:HG2	1.88	0.55
2:I:254:GLU:OE2	2:I:312:ARG:HD2	2.05	0.55
2:D:15:PHE:HE2	2:D:57:LEU:HB3	1.71	0.55
2:H:359:PHE:CZ	2:I:323:THR:HG23	2.41	0.55
1:F:64:ILE:HD12	1:F:96:GLN:HG2	1.89	0.55
2:C:309:ILE:HG22	2:C:313:MET:HG2	1.88	0.55
3:J:229:TRP:O	3:J:316:LEU:HD13	2.06	0.55
2:B:347:MET:CE	2:C:291:ARG:HH21	2.20	0.55
2:H:112:GLN:NE2	2:H:113:TYR:CE1	2.75	0.55
2:G:293:ALA:O	2:G:296:GLN:HB2	2.06	0.55
2:H:111:VAL:HG13	2:H:150:VAL:HG21	1.89	0.55
2:H:338:GLU:OE2	2:H:355:ARG:NH2	2.40	0.55
3:J:176:LEU:HD11	3:J:201:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:48:LEU:HD13	3:J:140:TRP:CD1	2.42	0.55
2:D:341:TYR:CD1	2:D:341:TYR:N	2.73	0.55
2:H:297:LEU:CD2	6:P:25:LEU:HD12	2.38	0.54
2:D:93:ILE:HD11	2:D:107:LEU:HD21	1.89	0.54
1:F:97:LEU:HD13	1:F:126:TRP:CH2	2.42	0.54
2:B:344:ASP:HB3	2:B:347:MET:H	1.72	0.54
2:C:24:VAL:HG21	2:C:175:LEU:HD22	1.88	0.54
2:D:254:GLU:OE1	2:D:312:ARG:NH1	2.41	0.54
2:D:32:LEU:HD23	2:D:37:ILE:HD13	1.89	0.54
2:C:64:CYS:SG	2:C:66:THR:HG23	2.47	0.54
2:I:68:ILE:HD11	2:I:120:PHE:HE2	1.72	0.54
3:E:48:LEU:HD13	3:E:140:TRP:CD1	2.42	0.54
2:H:30:ASN:O	2:H:34:LEU:HB2	2.08	0.54
2:D:362:ARG:HG2	6:O:4:ARG:CZ	2.38	0.54
3:E:4:TYR:HB3	3:E:6:TRP:CZ2	2.43	0.54
2:C:359:PHE:CD2	6:O:9:LEU:HD21	2.43	0.54
2:H:175:LEU:HD23	2:H:175:LEU:N	2.23	0.54
2:H:359:PHE:CE2	2:I:323:THR:HG23	2.43	0.54
6:P:9:LEU:HD12	6:P:16:GLN:NE2	2.22	0.54
1:A:305:LEU:HD13	1:A:327:LEU:HD21	1.90	0.54
1:A:213:THR:H	1:A:216:HIS:CD2	2.25	0.54
1:F:26:ASN:ND2	1:F:140:GLN:OE1	2.41	0.54
3:E:46:ARG:CD	3:E:68:MET:HG2	2.36	0.54
2:B:343:PRO:HG3	2:C:286:LEU:CB	2.37	0.54
2:H:344:ASP:HB3	2:H:347:MET:HB2	1.90	0.54
3:J:179:GLU:CB	3:J:202:LEU:HD11	2.38	0.54
1:F:172:TYR:HH	1:F:231:HIS:CE1	2.25	0.54
2:C:30:ASN:O	2:C:34:LEU:HB2	2.07	0.54
3:E:152:LEU:HD12	3:E:153:ALA:H	1.73	0.54
1:F:13:LEU:HD13	1:F:38:VAL:HG22	1.89	0.54
3:E:88:LEU:HD23	3:E:120:LEU:CD2	2.36	0.54
3:E:253:MET:HG3	3:E:253:MET:O	2.08	0.54
2:I:68:ILE:HD11	2:I:120:PHE:CE2	2.43	0.54
2:B:158:ASP:OD2	2:B:161:LYS:HE2	2.07	0.54
1:A:21:TYR:CD1	1:A:135:VAL:HB	2.43	0.54
1:F:71:MET:HB2	1:F:105:HIS:HE1	1.72	0.54
2:C:21:GLN:OE1	2:C:21:GLN:HA	2.08	0.54
2:G:101:VAL:HG22	2:G:135:SER:N	2.22	0.54
1:A:64:ILE:HD12	1:A:96:GLN:HG2	1.88	0.54
2:C:44:SER:CB	2:C:159:PRO:HG3	2.37	0.54
2:D:344:ASP:HB2	2:D:347:MET:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:ILE:HD13	2:D:316:LEU:HB3	1.90	0.54
2:I:56:ARG:HD3	2:I:92:GLU:OE1	2.07	0.54
2:C:290:HIS:CE1	2:C:294:MET:CE	2.91	0.54
2:C:49:VAL:HG11	2:C:176:LYS:O	2.08	0.54
1:F:267:THR:HB	1:F:268:PRO:CD	2.36	0.54
2:I:10:TRP:CE2	2:I:190:ILE:HG23	2.43	0.54
2:H:244:LEU:N	2:H:244:LEU:HD12	2.12	0.54
2:G:130:MET:CE	2:H:134:HIS:ND1	2.71	0.54
2:H:353:LEU:O	2:H:356:ALA:HB3	2.08	0.54
3:E:10:ASP:OD2	3:E:164:LEU:HD12	2.07	0.54
2:C:223:GLN:HB3	2:D:171:LEU:HD22	1.90	0.54
6:O:20:ARG:NH1	6:O:21:ARG:NH2	2.56	0.54
2:I:292:ILE:HG22	2:I:325:ILE:CD1	2.38	0.54
3:J:182:MET:HB2	3:J:187:LEU:HD21	1.89	0.53
2:B:24:VAL:HG22	2:B:173:PHE:HB3	1.89	0.53
2:C:246:ASP:HB3	2:C:309:ILE:CD1	2.36	0.53
3:E:259:HIS:ND1	3:J:259:HIS:ND1	2.53	0.53
2:D:68:ILE:HD11	2:D:120:PHE:HE2	1.72	0.53
2:I:215:ARG:HH11	2:I:215:ARG:CG	2.21	0.53
3:E:121:THR:HG22	3:E:122:ASP:H	1.74	0.53
2:C:344:ASP:HB3	2:C:347:MET:HB2	1.90	0.53
4:M:6:DT:H2"	4:M:7:DA:C8	2.43	0.53
2:B:260:ASN:ND2	2:B:263:ARG:HB2	2.24	0.53
2:D:24:VAL:HG21	2:D:175:LEU:CD2	2.39	0.53
3:E:35:MET:HE3	3:E:164:LEU:HG	1.89	0.53
3:E:179:GLU:CB	3:E:202:LEU:HD11	2.38	0.53
2:I:5:VAL:HG13	2:I:222:ASP:OD2	2.07	0.53
3:J:152:LEU:HD12	3:J:153:ALA:H	1.73	0.53
2:D:122:VAL:HG12	2:D:122:VAL:O	2.08	0.53
2:B:253:VAL:HG12	2:B:316:LEU:HD21	1.91	0.53
2:C:112:GLN:NE2	2:C:113:TYR:CE1	2.74	0.53
2:C:282:LEU:O	2:C:286:LEU:HD12	2.08	0.53
2:G:228:GLY:HA3	2:G:231:GLN:O	2.08	0.53
2:D:68:ILE:HD11	2:D:120:PHE:CE2	2.43	0.53
2:I:215:ARG:HG2	3:J:157:SER:O	2.08	0.53
1:A:71:MET:HB2	1:A:105:HIS:HE1	1.74	0.53
3:J:292:ASP:HB3	3:J:315:LEU:CD1	2.37	0.53
2:D:292:ILE:HG22	2:D:325:ILE:CD1	2.38	0.53
1:F:188:LEU:HD13	1:F:197:LEU:HD13	1.90	0.53
2:D:47:ARG:O	2:D:47:ARG:HG2	2.07	0.53
2:C:297:LEU:HD23	6:O:25:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:HD13	2:D:122:VAL:HG11	1.89	0.53
2:H:290:HIS:CE1	2:H:294:MET:CE	2.92	0.53
2:H:297:LEU:CD2	6:P:25:LEU:HA	2.38	0.53
1:A:21:TYR:CE1	1:A:135:VAL:HB	2.44	0.53
2:G:51:LYS:CB	7:G:406:ADP:O2B	2.53	0.53
2:B:338:GLU:C	2:B:340:PRO:HD2	2.28	0.53
3:E:270:VAL:HG23	3:E:270:VAL:O	2.08	0.53
2:H:49:VAL:HG11	2:H:176:LYS:O	2.09	0.53
3:J:68:MET:HE2	3:J:68:MET:HA	1.90	0.53
2:G:240:MET:O	2:G:243:THR:HB	2.09	0.53
1:F:296:THR:HG23	1:F:299:ARG:NH1	2.23	0.53
3:E:179:GLU:HB3	3:E:202:LEU:HD11	1.90	0.53
1:A:43:ALA:HA	1:A:47:PHE:O	2.09	0.53
2:G:-5:LEU:N	2:G:-5:LEU:HD23	2.23	0.53
2:C:353:LEU:O	2:C:356:ALA:HB3	2.07	0.53
2:H:51:LYS:N	7:H:408:ADP:O2B	2.41	0.53
3:J:179:GLU:HB3	3:J:202:LEU:HD11	1.90	0.53
2:I:292:ILE:O	2:I:296:GLN:HG3	2.08	0.53
2:C:214:LEU:HD12	2:C:214:LEU:O	2.09	0.53
2:G:292:ILE:CD1	2:G:316:LEU:HD23	2.38	0.53
2:I:327:LEU:CD2	6:P:12:LEU:HG	2.38	0.53
2:G:-8:LEU:O	2:G:-5:LEU:HG	2.09	0.53
2:H:178:LEU:CD1	2:H:214:LEU:HB2	2.39	0.53
2:C:234:THR:O	2:C:238:SER:OG	2.25	0.53
1:F:47:PHE:CZ	1:F:77:ARG:HD3	2.44	0.53
2:H:342:ALA:HB1	2:H:343:PRO:HD2	1.90	0.53
2:H:60:LYS:NZ	2:H:83:GLU:HG3	2.24	0.53
3:E:182:MET:HG3	3:E:205:PHE:CD1	2.44	0.52
1:A:29:LEU:HD23	1:A:178:LEU:HB3	1.91	0.52
3:E:213:ARG:HH21	3:E:267:ASN:HD22	1.55	0.52
1:A:237:ARG:HG3	1:A:321:TRP:CE2	2.44	0.52
2:B:291:ARG:CG	2:B:306:MET:HE3	2.30	0.52
2:B:292:ILE:HD13	2:B:316:LEU:HD23	1.90	0.52
2:C:137:ASN:HA	2:C:140:LEU:HG	1.91	0.52
1:A:223:MET:HG3	1:A:285:MET:HG3	1.91	0.52
2:D:29:ALA:CB	2:D:70:ALA:HB1	2.39	0.52
2:G:126:ASP:HB3	2:H:141:LYS:HD2	1.92	0.52
2:C:202:ALA:HB1	2:C:237:VAL:HG21	1.90	0.52
2:H:367:GLU:CG	2:H:368:PRO:HD2	2.30	0.52
2:H:147:PRO:HD2	2:H:150:VAL:HB	1.92	0.52
2:I:61:GLY:CA	2:I:72:PRO:HG3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG21	4:K:5:DT:C7	2.39	0.52
2:C:22:GLU:O	2:C:26:THR:HB	2.08	0.52
3:J:86:ASN:O	3:J:119:LEU:HD22	2.09	0.52
2:H:213:SER:HB3	2:H:216:ASP:HB2	1.89	0.52
1:A:42:ALA:O	1:A:47:PHE:HB2	2.10	0.52
1:A:192:TRP:CZ2	1:A:201:ARG:HG2	2.44	0.52
2:D:29:ALA:HB1	2:D:70:ALA:HB1	1.89	0.52
2:B:178:LEU:HD12	2:B:214:LEU:HB2	1.92	0.52
2:H:44:SER:CB	2:H:159:PRO:HG3	2.38	0.52
6:O:26:GLN:O	6:O:28:GLU:N	2.43	0.52
2:G:354:LEU:HD21	2:H:297:LEU:HB2	1.92	0.52
6:P:25:LEU:O	6:P:26:GLN:C	2.47	0.52
3:J:4:TYR:HB3	3:J:6:TRP:CZ2	2.45	0.52
3:E:182:MET:HB2	3:E:187:LEU:HD21	1.91	0.52
1:F:24:LEU:HD11	1:F:117:LEU:HD11	1.90	0.52
2:H:309:ILE:HG22	2:H:313:MET:HG2	1.91	0.52
3:J:35:MET:HG2	3:J:197:SER:HB3	1.90	0.52
2:C:224:ALA:HA	2:C:240:MET:HE1	1.91	0.52
1:F:314:GLN:OE1	3:J:303:VAL:CG2	2.57	0.52
2:H:130:MET:CE	2:I:134:HIS:CD2	2.92	0.52
4:M:12:DC:H2'	4:M:13:DC:O5'	2.10	0.52
1:F:261:LYS:HE2	1:F:293:LEU:O	2.09	0.52
1:A:280:GLN:HA	1:A:283:ARG:HG3	1.91	0.52
3:E:19:GLN:HG2	3:E:47:TYR:OH	2.10	0.52
2:B:147:PRO:HB2	2:B:150:VAL:CG2	2.39	0.52
2:I:347:MET:HE1	3:J:250:THR:HG22	1.92	0.52
2:B:161:LYS:HE3	2:C:133:ARG:NH1	2.24	0.52
3:E:199:GLY:HA2	3:E:202:LEU:HB2	1.92	0.52
1:F:177:ASN:HD21	1:F:180:ALA:HB2	1.73	0.52
2:H:359:PHE:CD2	6:P:9:LEU:HD21	2.45	0.52
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.91	0.52
2:G:223:GLN:HG2	2:G:240:MET:SD	2.50	0.52
2:H:224:ALA:HA	2:H:240:MET:HE1	1.91	0.52
1:A:36:ASP:CG	2:B:169:ARG:HH22	2.13	0.52
2:D:111:VAL:HG13	2:D:150:VAL:HG21	1.92	0.52
1:A:47:PHE:CZ	1:A:77:ARG:HD3	2.43	0.52
1:F:64:ILE:HA	1:F:67:LEU:HD12	1.92	0.52
2:D:42:LEU:HA	2:D:154:LEU:O	2.10	0.52
1:F:280:GLN:HA	1:F:283:ARG:HG3	1.91	0.52
1:A:181:LEU:O	1:A:184:ALA:HB3	2.10	0.52
2:C:197:ALA:HB3	2:C:231:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:THR:CG2	6:O:8:GLN:OE1	2.59	0.51
2:C:346:ARG:O	2:C:347:MET:C	2.47	0.51
1:A:319:SER:O	1:A:321:TRP:N	2.43	0.51
3:J:126:ASN:HA	3:J:129:LEU:HG	1.93	0.51
2:D:362:ARG:HG2	6:O:4:ARG:NE	2.25	0.51
2:H:53:SER:OG	7:H:408:ADP:O1A	2.27	0.51
2:I:74:GLY:HA2	2:I:79:CYS:CB	2.40	0.51
3:E:82:GLU:HA	3:E:82:GLU:OE1	2.10	0.51
3:E:46:ARG:NH1	3:E:69:GLN:HG3	2.26	0.51
1:F:9:LEU:HD11	1:F:13:LEU:HD21	1.92	0.51
2:I:344:ASP:HB2	2:I:347:MET:H	1.75	0.51
2:I:265:MET:CE	3:J:257:LYS:HD3	2.41	0.51
1:F:181:LEU:O	1:F:184:ALA:HB3	2.09	0.51
2:I:261:GLY:HA2	2:I:357:LEU:HD21	1.93	0.51
1:F:236:LEU:HD13	1:F:246:LEU:HD21	1.92	0.51
2:D:6:LEU:N	2:D:6:LEU:HD12	2.12	0.51
1:F:55:ILE:CG2	1:F:93:ILE:HD13	2.41	0.51
1:A:81:LEU:HD13	1:A:111:ILE:HG22	1.92	0.51
2:B:101:VAL:HG22	2:B:135:SER:N	2.26	0.51
2:H:254:GLU:OE2	2:H:312:ARG:CD	2.59	0.51
1:A:318:GLN:CD	1:A:318:GLN:H	2.14	0.51
2:H:295:VAL:HG22	2:H:302:LEU:HB2	1.92	0.51
3:J:52:GLN:N	3:J:53:PRO:HD3	2.26	0.51
3:J:20:ALA:HB1	3:J:22:ARG:HG3	1.93	0.51
2:B:240:MET:O	2:B:243:THR:HB	2.11	0.51
1:A:2:ILE:HG13	1:A:18:ARG:NH1	2.25	0.51
2:B:51:LYS:CB	7:B:400:ADP:O2B	2.55	0.51
2:D:362:ARG:O	2:D:363:MET:CG	2.57	0.51
3:J:182:MET:HG3	3:J:205:PHE:CD1	2.46	0.51
2:I:24:VAL:HG21	2:I:175:LEU:CD2	2.39	0.51
3:J:35:MET:HE3	3:J:164:LEU:HG	1.93	0.51
1:F:292:ARG:HH12	1:F:293:LEU:HD21	1.75	0.51
3:J:112:VAL:HB	3:J:141:PHE:CD1	2.46	0.51
2:G:57:LEU:HD23	2:G:60:LYS:HD2	1.92	0.51
1:F:42:ALA:O	1:F:47:PHE:HB2	2.11	0.51
2:D:302:LEU:HD11	2:D:306:MET:CG	2.39	0.51
2:H:282:LEU:HG	2:H:349:VAL:HG22	1.92	0.51
3:J:207:GLY:C	3:J:209:ASN:H	2.12	0.51
2:C:254:GLU:OE2	2:C:312:ARG:CD	2.59	0.51
1:A:118:SER:OG	1:A:121:GLN:HG2	2.10	0.51
2:D:268:ILE:HG23	2:D:278:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HE1	4:K:3:DT:C6	2.29	0.51
2:B:341:TYR:CE1	2:C:337:LYS:HE3	2.46	0.51
2:I:252:LEU:HD13	2:I:285:MET:HE1	1.93	0.51
3:E:34:GLY:HA3	3:E:200:ALA:HB2	1.92	0.51
1:F:118:SER:OG	1:F:121:GLN:HG2	2.11	0.51
2:I:341:TYR:N	2:I:341:TYR:CD1	2.78	0.51
4:M:9:DA:H2''	4:M:10:DG:O5'	2.11	0.51
2:H:115:PRO:CD	2:H:149:HIS:HD2	2.19	0.51
1:F:78:GLN:HG3	1:F:108:LEU:HD22	1.93	0.51
3:E:121:THR:CG2	3:E:122:ASP:N	2.74	0.51
2:B:46:THR:HG22	2:B:47:ARG:HD3	1.92	0.51
2:G:309:ILE:HG22	2:G:313:MET:HG2	1.92	0.51
1:A:194:ASP:HB3	1:A:196:LYS:HG2	1.94	0.50
1:F:192:TRP:CZ2	1:F:201:ARG:HG2	2.46	0.50
2:C:307:ALA:C	2:C:309:ILE:H	2.14	0.50
2:H:340:PRO:HB2	2:H:341:TYR:CD1	2.46	0.50
2:G:321:PRO:HB2	2:G:324:ASP:HB2	1.93	0.50
2:I:145:GLU:N	2:I:146:PRO:HD3	2.26	0.50
1:F:244:VAL:HG21	4:M:5:DT:C7	2.41	0.50
1:A:237:ARG:O	1:A:240:GLY:N	2.41	0.50
1:F:43:ALA:HA	1:F:47:PHE:O	2.12	0.50
1:A:267:THR:HB	1:A:268:PRO:CD	2.40	0.50
1:F:81:LEU:HD13	1:F:111:ILE:HG22	1.94	0.50
2:C:113:TYR:N	2:C:113:TYR:CD1	2.78	0.50
2:H:112:GLN:HG3	2:H:113:TYR:CD1	2.47	0.50
3:E:35:MET:HG2	3:E:197:SER:HB3	1.91	0.50
3:E:4:TYR:HB3	3:E:6:TRP:CH2	2.46	0.50
1:A:77:ARG:NH1	1:A:106:ASP:HB3	2.27	0.50
2:I:29:ALA:CB	2:I:70:ALA:HB1	2.41	0.50
1:F:282:ARG:HD3	1:F:285:MET:CE	2.42	0.50
2:G:128:VAL:HG12	2:G:156:THR:HB	1.92	0.50
2:I:100:LYS:O	2:I:104:THR:HG23	2.12	0.50
2:D:268:ILE:HD11	2:D:353:LEU:CD1	2.31	0.50
1:A:215:PHE:CE1	4:K:3:DT:C6	3.00	0.50
2:D:128:VAL:C	2:D:130:MET:H	2.13	0.50
2:I:309:ILE:O	2:I:310:GLU:C	2.50	0.50
3:J:253:MET:O	3:J:253:MET:HG3	2.11	0.50
2:I:32:LEU:HD23	2:I:37:ILE:HD13	1.94	0.50
1:A:174:TYR:HB2	1:A:181:LEU:HD13	1.94	0.50
3:E:112:VAL:HB	3:E:141:PHE:CD1	2.46	0.50
2:H:21:GLN:OE1	2:H:21:GLN:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LEU:O	2:B:292:ILE:HG13	2.11	0.50
2:H:334:ILE:O	2:H:338:GLU:HG3	2.11	0.50
2:I:29:ALA:HB1	2:I:70:ALA:HB1	1.93	0.50
2:G:178:LEU:CD1	2:G:214:LEU:HD22	2.41	0.50
2:D:42:LEU:HD12	2:D:154:LEU:O	2.11	0.50
2:H:197:ALA:HB3	2:H:231:GLN:HG2	1.94	0.50
2:I:91:ILE:HD12	2:I:123:TYR:CE2	2.46	0.50
2:D:49:VAL:CG1	2:D:49:VAL:O	2.60	0.50
3:E:20:ALA:HB1	3:E:22:ARG:HG3	1.90	0.50
3:E:253:MET:HE2	3:E:290:LEU:HD21	1.93	0.50
3:E:176:LEU:HD11	3:E:201:ALA:HB1	1.94	0.50
1:A:97:LEU:HD12	1:A:126:TRP:CZ2	2.47	0.50
2:G:111:VAL:HA	2:G:123:TYR:OH	2.11	0.50
2:G:32:LEU:HD21	2:G:62:LEU:HD23	1.94	0.50
3:J:88:LEU:HD23	3:J:120:LEU:CD2	2.41	0.50
1:A:236:LEU:HD13	1:A:246:LEU:HD21	1.94	0.50
1:F:41:VAL:O	1:F:45:GLN:HG2	2.12	0.50
2:C:342:ALA:HB1	2:C:343:PRO:HD2	1.93	0.50
2:D:215:ARG:HE	7:D:404:ADP:H5'1	1.77	0.50
1:F:77:ARG:NH1	1:F:106:ASP:HB3	2.26	0.50
2:D:101:VAL:CG2	2:D:134:HIS:HB3	2.42	0.50
2:B:344:ASP:HB3	2:B:347:MET:HB2	1.93	0.50
2:B:128:VAL:HG12	2:B:156:THR:HB	1.93	0.50
3:E:94:ARG:HA	3:E:97:THR:OG1	2.12	0.50
2:I:101:VAL:CG2	2:I:134:HIS:HB3	2.42	0.49
1:A:215:PHE:HE1	4:K:3:DT:C7	2.25	0.49
2:I:306:MET:O	2:I:307:ALA:C	2.50	0.49
2:D:363:MET:SD	3:J:221:ALA:HB1	2.51	0.49
2:G:252:LEU:CD2	2:G:267:LEU:HB2	2.42	0.49
1:A:29:LEU:HD22	1:A:179:LEU:HA	1.93	0.49
1:F:142:PRO:HD3	1:F:178:LEU:HD11	1.93	0.49
2:I:362:ARG:HG2	6:P:4:ARG:NH2	2.27	0.49
2:B:321:PRO:HB2	2:B:324:ASP:HB2	1.94	0.49
3:E:148:PRO:O	3:E:151:LEU:HB2	2.11	0.49
2:I:215:ARG:CG	3:J:157:SER:O	2.59	0.49
3:E:2:ARG:CD	3:E:4:TYR:CE1	2.83	0.49
4:K:9:DA:H2''	4:K:10:DG:O5'	2.12	0.49
1:F:53:PHE:CD1	1:F:67:LEU:HD21	2.47	0.49
3:J:68:MET:CE	3:J:68:MET:HA	2.42	0.49
3:E:46:ARG:HH12	3:E:69:GLN:HG3	1.76	0.49
6:P:20:ARG:NH1	6:P:21:ARG:NH2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:ASN:ND2	1:F:180:ALA:HB2	2.27	0.49
2:B:286:LEU:HD21	2:B:333:LEU:N	2.26	0.49
2:C:4:GLN:OE1	2:C:4:GLN:HA	2.10	0.49
2:D:75:VAL:O	2:D:75:VAL:HG12	2.12	0.49
2:B:302:LEU:HD12	2:B:310:GLU:HG3	1.94	0.49
2:I:152:PHE:O	2:I:153:LEU:HD23	2.13	0.49
2:I:75:VAL:O	2:I:75:VAL:HG12	2.12	0.49
2:C:47:ARG:NH1	2:C:216:ASP:OD2	2.45	0.49
2:H:341:TYR:CE2	2:I:337:LYS:HG3	2.47	0.49
2:D:291:ARG:O	2:D:294:MET:HB2	2.12	0.49
2:D:74:GLY:HA2	2:D:79:CYS:CB	2.42	0.49
2:B:13:GLN:O	2:B:57:LEU:HD21	2.12	0.49
3:E:249:ALA:HB2	3:E:293:VAL:HG11	1.94	0.49
2:B:268:ILE:HD13	2:B:350:GLU:HG2	1.95	0.49
2:H:229:ASP:CB	2:I:30:ASN:HD21	2.25	0.49
2:D:190:ILE:HD12	2:D:218:LEU:HD21	1.93	0.49
3:E:213:ARG:HH11	3:E:213:ARG:HG2	1.77	0.49
2:H:223:GLN:HB3	2:I:171:LEU:HD22	1.95	0.49
1:A:41:VAL:O	1:A:45:GLN:HG2	2.12	0.49
2:C:213:SER:HB3	2:C:216:ASP:HB2	1.94	0.49
2:I:324:ASP:OD1	6:P:8:GLN:NE2	2.45	0.49
1:F:2:ILE:HG13	1:F:18:ARG:NH1	2.27	0.49
2:D:69:THR:HG21	2:D:72:PRO:HA	1.94	0.49
2:D:357:LEU:HD23	3:E:260:HIS:CE1	2.47	0.49
3:J:80:ALA:HB1	3:J:81:PRO:CD	2.41	0.49
2:G:15:PHE:CE2	2:G:57:LEU:HB3	2.47	0.49
2:B:15:PHE:HE2	2:B:57:LEU:HB3	1.78	0.49
2:G:92:GLU:HG3	2:G:124:LEU:HG	1.93	0.49
5:N:4:DG:H2''	5:N:5:DC:O5'	2.13	0.49
3:E:29:ILE:O	3:E:144:ALA:HA	2.13	0.49
2:H:144:GLU:HG2	2:H:145:GLU:HG3	1.95	0.49
2:G:286:LEU:HD21	2:G:333:LEU:N	2.28	0.49
3:E:4:TYR:CB	3:E:6:TRP:CZ2	2.95	0.49
2:G:51:LYS:N	7:G:406:ADP:O2B	2.46	0.49
2:H:229:ASP:HB2	2:I:30:ASN:HD21	1.78	0.49
2:I:291:ARG:O	2:I:294:MET:HB2	2.13	0.49
2:B:260:ASN:HD22	2:B:263:ARG:CB	2.25	0.49
2:I:12:PRO:HG3	7:I:410:ADP:C2	2.47	0.49
2:C:101:VAL:CG2	4:K:12:DC:H5''	2.43	0.49
2:B:126:ASP:HB3	2:C:141:LYS:HD2	1.95	0.49
3:J:148:PRO:O	3:J:151:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:LEU:HD21	3:J:306:ILE:CD1	2.43	0.49
2:C:5:VAL:HG12	2:C:8:ARG:H	1.78	0.49
2:I:122:VAL:O	2:I:122:VAL:HG12	2.13	0.49
1:A:55:ILE:HD11	1:A:82:LEU:HD22	1.95	0.49
1:F:237:ARG:HG3	1:F:321:TRP:CD2	2.48	0.49
2:G:344:ASP:HB3	2:G:347:MET:HB2	1.93	0.49
1:F:73:LEU:HD11	1:F:105:HIS:CD2	2.47	0.49
2:H:254:GLU:OE2	2:H:312:ARG:HD2	2.12	0.49
4:K:6:DT:H2''	4:K:7:DA:C8	2.47	0.49
3:E:292:ASP:CG	3:E:318:ARG:HH21	2.16	0.48
1:A:147:LEU:HD23	1:A:171:CYS:SG	2.53	0.48
2:H:90:LEU:O	2:H:90:LEU:HG	2.13	0.48
2:C:243:THR:HG22	2:C:244:LEU:O	2.12	0.48
2:G:291:ARG:HG2	2:G:306:MET:HE1	1.91	0.48
3:J:224:VAL:CB	3:J:225:PRO:HD3	2.37	0.48
2:B:250:LEU:HA	2:B:288:LEU:HD13	1.95	0.48
2:C:137:ASN:H	2:C:137:ASN:ND2	2.10	0.48
3:J:99:LYS:CD	3:J:105:ARG:NH2	2.76	0.48
2:G:13:GLN:O	2:G:57:LEU:HD21	2.13	0.48
1:A:296:THR:O	1:A:300:GLN:HG3	2.13	0.48
2:B:354:LEU:HD21	2:C:297:LEU:HB2	1.95	0.48
1:A:150:TRP:CZ3	1:A:178:LEU:HD22	2.49	0.48
2:C:112:GLN:HG3	2:C:113:TYR:CD1	2.48	0.48
2:H:307:ALA:O	2:H:309:ILE:N	2.46	0.48
2:G:214:LEU:O	2:G:217:ALA:HB3	2.14	0.48
3:J:14:LEU:HD21	3:J:162:HIS:ND1	2.27	0.48
1:A:9:LEU:HD11	1:A:13:LEU:HD21	1.95	0.48
2:G:20:GLY:HA2	2:G:22:GLU:OE2	2.13	0.48
2:G:101:VAL:HG21	2:G:134:HIS:HB2	1.95	0.48
2:H:307:ALA:C	2:H:309:ILE:H	2.15	0.48
1:A:259:ASN:O	1:A:263:GLN:HG3	2.14	0.48
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.60	0.48
3:E:114:VAL:CB	3:E:143:LEU:CD2	2.82	0.48
2:H:290:HIS:CE1	2:H:294:MET:HE2	2.48	0.48
2:I:327:LEU:HD11	6:P:8:GLN:CG	2.38	0.48
2:H:140:LEU:HD22	2:H:169:ARG:NH1	2.28	0.48
2:I:302:LEU:HD11	2:I:306:MET:CG	2.37	0.48
1:A:196:LYS:O	1:A:201:ARG:NH1	2.46	0.48
2:G:250:LEU:HA	2:G:288:LEU:HD13	1.94	0.48
3:E:259:HIS:HD1	3:J:259:HIS:CE1	2.30	0.48
2:G:5:VAL:HG21	2:H:39:HIS:ND1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:163:TYR:CE2	3:J:165:ALA:HB2	2.48	0.48
2:H:108:LEU:O	2:H:109:ASP:C	2.51	0.48
2:H:290:HIS:CE1	2:H:294:MET:HE1	2.49	0.48
2:C:147:PRO:HD2	2:C:150:VAL:HB	1.95	0.48
2:B:285:MET:O	2:B:288:LEU:HB2	2.14	0.48
1:F:305:LEU:HD13	1:F:327:LEU:HD21	1.96	0.48
1:F:150:TRP:CZ3	1:F:178:LEU:HD22	2.48	0.48
2:D:186:GLN:NE2	2:D:190:ILE:HD11	2.29	0.48
2:B:15:PHE:CE2	2:B:57:LEU:HB3	2.48	0.48
1:F:310:LEU:CD2	3:J:306:ILE:HD12	2.43	0.48
5:L:6:DC:H2''	5:L:7:DT:O5'	2.13	0.48
3:E:300:LEU:HA	3:E:300:LEU:HD23	1.66	0.48
3:J:170:GLN:HA	3:J:170:GLN:OE1	2.13	0.48
2:I:47:ARG:HG3	3:J:157:SER:OG	2.13	0.48
1:A:53:PHE:CE2	1:A:67:LEU:HD11	2.49	0.48
3:J:33:PRO:C	3:J:35:MET:H	2.16	0.48
2:C:15:PHE:HE1	2:C:57:LEU:HB3	1.78	0.48
2:I:356:ALA:O	2:I:359:PHE:HD2	1.97	0.48
2:C:290:HIS:NE2	2:C:294:MET:CE	2.76	0.48
4:M:10:DG:H2''	4:M:11:DG:O5'	2.14	0.48
1:A:73:LEU:H	1:A:73:LEU:HD12	1.79	0.48
2:H:137:ASN:HD22	2:H:137:ASN:H	1.61	0.48
1:A:53:PHE:CD1	1:A:67:LEU:HD21	2.48	0.48
2:I:311:LEU:HD12	2:I:311:LEU:HA	1.54	0.48
2:C:307:ALA:O	2:C:309:ILE:N	2.47	0.48
3:J:76:TYR:HD1	3:J:111:VAL:HG23	1.79	0.48
2:C:254:GLU:OE2	2:C:312:ARG:HD2	2.14	0.48
2:D:145:GLU:N	2:D:146:PRO:HD3	2.28	0.48
2:I:15:PHE:CE2	2:I:57:LEU:HB3	2.49	0.48
2:B:179:ASP:CB	2:B:182:GLN:HG3	2.31	0.48
2:H:23:HIS:HE1	2:H:174:HIS:O	1.97	0.48
2:D:311:LEU:HA	2:D:311:LEU:HD12	1.57	0.48
1:A:27:ASP:O	1:A:31:LEU:HG	2.14	0.48
1:A:222:LEU:HD12	1:A:285:MET:HE3	1.96	0.48
2:D:324:ASP:OD1	6:O:8:GLN:NE2	2.47	0.48
1:A:48:GLU:HG3	1:A:49:GLU:N	2.29	0.48
2:H:47:ARG:HH11	2:I:164:VAL:CG2	2.27	0.48
1:F:53:PHE:CE2	1:F:67:LEU:HD11	2.49	0.48
2:H:338:GLU:HB3	2:I:333:LEU:HD21	1.96	0.48
2:I:347:MET:O	2:I:351:MET:HG3	2.14	0.48
2:B:264:VAL:HG21	2:B:357:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:CYS:O	2:C:75:VAL:HG13	2.13	0.48
2:B:325:ILE:O	2:B:326:GLN:C	2.51	0.48
2:C:316:LEU:HD23	2:C:320:ILE:HD11	1.96	0.48
3:E:126:ASN:HA	3:E:129:LEU:HG	1.94	0.48
1:A:55:ILE:CG2	1:A:93:ILE:HD13	2.44	0.47
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.96	0.47
1:F:188:LEU:CD1	1:F:202:VAL:HG22	2.44	0.47
2:G:10:TRP:CE2	2:G:190:ILE:HG23	2.49	0.47
1:A:261:LYS:HE2	1:A:293:LEU:O	2.13	0.47
3:J:90:VAL:HG13	3:J:91:ASP:N	2.29	0.47
2:H:5:VAL:HG12	2:H:8:ARG:H	1.78	0.47
3:E:170:GLN:HA	3:E:170:GLN:OE1	2.14	0.47
2:B:350:GLU:CB	2:C:294:MET:HE1	2.28	0.47
3:J:29:ILE:O	3:J:144:ALA:HA	2.14	0.47
2:B:305:ASP:OD1	2:B:306:MET:N	2.47	0.47
2:D:323:THR:HG22	6:O:8:GLN:CD	2.34	0.47
2:B:24:VAL:HG21	2:B:175:LEU:HD22	1.94	0.47
3:E:68:MET:HA	3:E:68:MET:CE	2.44	0.47
3:J:51:GLN:OE1	3:J:106:LEU:HD21	2.15	0.47
2:I:42:LEU:HA	2:I:154:LEU:O	2.13	0.47
3:E:147:GLU:HG3	3:E:147:GLU:O	2.13	0.47
1:A:2:ILE:HG13	1:A:18:ARG:HH12	1.79	0.47
2:G:305:ASP:OD1	2:G:306:MET:N	2.47	0.47
2:H:128:VAL:HG13	2:H:162:LEU:HD21	1.95	0.47
2:C:268:ILE:HD11	2:C:353:LEU:CD1	2.40	0.47
3:E:222:TYR:O	3:E:225:PRO:HD2	2.14	0.47
2:D:91:ILE:HD12	2:D:123:TYR:CE2	2.49	0.47
2:I:49:VAL:CG1	2:I:49:VAL:O	2.62	0.47
2:D:32:LEU:HD23	2:D:37:ILE:HD11	1.97	0.47
1:F:147:LEU:HD23	1:F:171:CYS:SG	2.54	0.47
1:A:177:ASN:HD21	1:A:180:ALA:HB2	1.79	0.47
3:E:229:TRP:O	3:E:316:LEU:HD13	2.14	0.47
4:M:4:DT:H2'	4:M:4:DT:O5'	2.14	0.47
2:C:147:PRO:HB2	2:C:149:HIS:ND1	2.29	0.47
2:H:128:VAL:HG22	2:H:128:VAL:O	2.14	0.47
2:D:309:ILE:O	2:D:310:GLU:C	2.52	0.47
3:E:224:VAL:HG12	3:E:225:PRO:N	2.28	0.47
2:H:4:GLN:HA	2:H:4:GLN:OE1	2.13	0.47
2:I:306:MET:O	2:I:308:ALA:N	2.47	0.47
2:H:265:MET:HE1	2:I:294:MET:SD	2.54	0.47
1:A:142:PRO:HD3	1:A:178:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ALA:O	2:B:296:GLN:HB2	2.15	0.47
3:E:99:LYS:CD	3:E:105:ARG:NH2	2.77	0.47
2:B:178:LEU:CD1	2:B:214:LEU:HD22	2.44	0.47
5:N:1:DC:H1'	5:N:2:DT:H71	1.97	0.47
3:J:4:TYR:HB3	3:J:6:TRP:CH2	2.49	0.47
2:G:130:MET:HE3	2:H:134:HIS:ND1	2.30	0.47
2:H:144:GLU:HB2	2:H:169:ARG:NE	2.28	0.47
3:E:285:ARG:HH11	3:E:285:ARG:HG2	1.78	0.47
2:H:346:ARG:O	2:H:347:MET:C	2.51	0.47
3:J:297:ARG:O	3:J:301:MET:HG3	2.15	0.47
2:I:154:LEU:HA	2:I:154:LEU:HD23	1.59	0.47
3:J:324:GLN:OE1	3:J:325:PRO:HD3	2.15	0.47
2:B:350:GLU:OE1	2:C:290:HIS:HE1	1.98	0.47
1:A:98:LEU:CD2	1:A:126:TRP:HB3	2.42	0.47
2:I:128:VAL:C	2:I:130:MET:H	2.16	0.47
1:F:2:ILE:HG13	1:F:18:ARG:HH12	1.80	0.47
2:H:140:LEU:HD22	2:H:169:ARG:CZ	2.45	0.47
2:C:128:VAL:HG13	2:C:162:LEU:HD21	1.96	0.47
2:D:306:MET:O	2:D:309:ILE:N	2.47	0.47
2:C:229:ASP:OD1	2:D:34:LEU:HD21	2.15	0.47
2:B:252:LEU:CD2	2:B:267:LEU:HB2	2.43	0.47
3:E:276:GLU:OE1	2:I:363:MET:SD	2.72	0.47
1:F:223:MET:HG3	1:F:285:MET:HG3	1.97	0.47
1:F:237:ARG:O	1:F:240:GLY:N	2.39	0.47
2:H:178:LEU:HD12	2:H:214:LEU:HB2	1.96	0.47
2:C:178:LEU:CD1	2:C:214:LEU:HB2	2.45	0.47
2:C:250:LEU:O	2:C:254:GLU:HG3	2.14	0.47
2:C:102:GLU:OE1	2:C:102:GLU:HA	2.15	0.47
2:H:260:ASN:OD1	2:H:260:ASN:C	2.51	0.47
2:C:299:PRO:C	2:C:301:ALA:H	2.18	0.47
2:D:196:ILE:HD12	2:D:225:ILE:HD13	1.96	0.47
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.75	0.47
4:K:4:DT:O5'	4:K:4:DT:H2'	2.14	0.47
1:A:78:GLN:HG3	1:A:108:LEU:HD22	1.97	0.47
2:G:24:VAL:HG21	2:G:175:LEU:HD22	1.96	0.47
2:I:291:ARG:O	2:I:294:MET:N	2.48	0.47
2:B:42:LEU:HD12	2:B:43:PHE:H	1.79	0.47
2:H:223:GLN:HG3	2:H:240:MET:HE1	1.97	0.47
2:I:221:THR:O	2:I:225:ILE:HG13	2.15	0.47
5:N:9:DT:H2''	5:N:10:DA:C8	2.50	0.47
1:F:143:GLU:O	1:F:145:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:CYS:SG	1:F:206:VAL:CG1	3.03	0.47
1:F:84:LEU:HD23	1:F:88:GLY:HA2	1.95	0.47
1:F:48:GLU:HG3	1:F:49:GLU:N	2.28	0.47
2:G:215:ARG:O	2:G:216:ASP:C	2.53	0.47
2:C:334:ILE:O	2:C:338:GLU:HG3	2.14	0.47
1:A:26:ASN:OD1	1:A:27:ASP:N	2.48	0.47
2:H:279:GLU:O	2:H:283:VAL:HG23	2.14	0.47
2:C:244:LEU:HD12	2:C:244:LEU:N	2.13	0.47
3:J:4:TYR:CB	3:J:6:TRP:CZ2	2.97	0.47
1:F:55:ILE:HD11	1:F:82:LEU:HD22	1.96	0.47
2:H:23:HIS:CE1	2:H:24:VAL:HG23	2.50	0.47
1:A:67:LEU:O	1:A:70:ALA:HB3	2.15	0.47
2:B:91:ILE:HD13	2:B:123:TYR:CE2	2.50	0.47
2:D:59:ALA:O	2:D:60:LYS:C	2.54	0.47
3:J:244:ARG:HG2	3:J:247:TRP:CZ3	2.50	0.47
2:C:260:ASN:OD1	2:C:260:ASN:C	2.54	0.47
2:H:368:PRO:HG2	2:I:319:THR:O	2.15	0.46
2:H:147:PRO:HB2	2:H:149:HIS:ND1	2.29	0.46
3:J:28:LEU:O	3:J:161:LEU:HD12	2.14	0.46
2:D:125:ILE:CD1	2:D:125:ILE:N	2.78	0.46
3:J:19:GLN:HG2	3:J:47:TYR:OH	2.15	0.46
2:B:94:ASP:O	2:B:96:ALA:N	2.49	0.46
2:H:124:LEU:HA	2:H:153:LEU:O	2.15	0.46
2:I:111:VAL:HG12	2:I:112:GLN:N	2.30	0.46
2:D:215:ARG:CG	2:D:215:ARG:HH11	2.28	0.46
2:I:101:VAL:N	4:M:10:DG:OP1	2.48	0.46
1:A:73:LEU:N	1:A:73:LEU:HD12	2.30	0.46
2:I:128:VAL:HG22	2:I:128:VAL:O	2.13	0.46
1:F:73:LEU:HD11	1:F:105:HIS:NE2	2.30	0.46
2:B:51:LYS:N	7:B:400:ADP:O2B	2.48	0.46
1:F:194:ASP:HB3	1:F:196:LYS:HG2	1.95	0.46
2:B:91:ILE:HG22	2:B:93:ILE:CD1	2.46	0.46
2:H:246:ASP:HB3	2:H:309:ILE:CD1	2.43	0.46
2:C:347:MET:HG3	2:D:290:HIS:CE1	2.50	0.46
2:D:261:GLY:HA2	2:D:357:LEU:HD21	1.97	0.46
3:E:197:SER:OG	3:E:200:ALA:HB3	2.16	0.46
3:E:213:ARG:NH1	3:E:213:ARG:HG2	2.30	0.46
2:B:128:VAL:O	2:B:128:VAL:HG22	2.13	0.46
2:D:52:THR:OG1	2:D:126:ASP:OD1	2.33	0.46
3:E:264:GLN:HG2	3:E:264:GLN:O	2.12	0.46
2:B:111:VAL:HA	2:B:123:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:198:PRO:O	3:J:200:ALA:N	2.46	0.46
2:D:43:PHE:N	2:D:154:LEU:O	2.39	0.46
2:C:60:LYS:NZ	2:C:83:GLU:HG3	2.30	0.46
1:F:262:ARG:NH2	3:J:320:GLU:OE1	2.48	0.46
2:C:297:LEU:HD22	2:C:297:LEU:HA	1.56	0.46
2:H:101:VAL:HG21	4:M:12:DC:H5'	1.97	0.46
2:H:101:VAL:HG21	2:H:134:HIS:HB3	1.97	0.46
1:F:67:LEU:O	1:F:70:ALA:HB3	2.15	0.46
2:D:152:PHE:O	2:D:153:LEU:HD23	2.15	0.46
2:C:140:LEU:HD22	2:C:169:ARG:NH1	2.31	0.46
3:E:207:GLY:C	3:E:209:ASN:N	2.69	0.46
2:D:292:ILE:O	2:D:296:GLN:HG3	2.16	0.46
2:G:57:LEU:HD23	2:G:57:LEU:HA	1.66	0.46
2:D:18:VAL:HG11	2:D:25:LEU:HD11	1.96	0.46
6:O:25:LEU:O	6:O:26:GLN:C	2.53	0.46
1:F:215:PHE:HE1	4:M:3:DT:H72	1.80	0.46
2:B:78:ASN:O	2:B:82:ILE:HG13	2.16	0.46
2:G:250:LEU:HD23	2:G:312:ARG:NH2	2.30	0.46
2:I:12:PRO:HD3	7:I:410:ADP:H2'	1.97	0.46
2:B:228:GLY:HA3	2:B:231:GLN:O	2.16	0.46
2:C:140:LEU:HD23	2:C:166:ILE:HD13	1.97	0.46
2:H:339:LEU:HB3	2:H:340:PRO:HD3	1.98	0.46
3:E:51:GLN:OE1	3:E:106:LEU:HD21	2.16	0.46
3:E:20:ALA:HB3	3:E:22:ARG:HG3	1.97	0.46
2:G:296:GLN:C	2:G:297:LEU:HD12	2.35	0.46
1:F:230:LEU:HD13	2:G:301:ALA:HA	1.98	0.46
2:H:299:PRO:C	2:H:301:ALA:H	2.18	0.46
2:D:353:LEU:HD23	2:D:353:LEU:HA	1.70	0.46
2:G:50:GLY:O	2:G:51:LYS:C	2.54	0.46
1:F:308:THR:HG22	1:F:323:GLU:OE1	2.16	0.46
3:E:33:PRO:C	3:E:35:MET:H	2.18	0.46
2:G:189:HIS:O	2:G:192:ASN:HB2	2.16	0.46
3:E:80:ALA:HB1	3:E:81:PRO:CD	2.46	0.46
2:C:23:HIS:HE1	2:C:174:HIS:O	1.97	0.46
3:J:285:ARG:O	3:J:286:LEU:C	2.52	0.46
2:B:260:ASN:HD22	2:B:263:ARG:N	2.08	0.46
2:H:341:TYR:HB2	2:I:333:LEU:CD1	2.42	0.46
2:D:292:ILE:HG22	2:D:325:ILE:HD13	1.98	0.46
2:B:57:LEU:HD23	2:B:60:LYS:HD2	1.97	0.46
2:D:142:THR:O	2:D:146:PRO:HG3	2.15	0.46
2:B:10:TRP:CE2	2:B:190:ILE:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HD3	1:A:50:HIS:ND1	2.30	0.46
1:A:97:LEU:CD1	1:A:126:TRP:CH2	2.99	0.46
1:A:42:ALA:C	1:A:47:PHE:HB2	2.35	0.46
2:H:327:LEU:C	2:H:327:LEU:HD12	2.36	0.46
2:G:47:ARG:NH2	2:G:211:GLU:O	2.49	0.46
2:G:15:PHE:HE2	2:G:57:LEU:HB3	1.80	0.46
2:D:202:ALA:HB2	2:D:234:THR:HA	1.97	0.46
1:A:84:LEU:HD23	1:A:88:GLY:HA2	1.98	0.46
2:C:297:LEU:HD23	6:O:25:LEU:HD13	1.96	0.46
2:H:47:ARG:HD3	2:H:47:ARG:H	1.81	0.46
1:A:64:ILE:HA	1:A:67:LEU:HD12	1.97	0.46
3:E:76:TYR:HD1	3:E:111:VAL:HG23	1.81	0.46
2:H:202:ALA:HB1	2:H:237:VAL:HG21	1.98	0.46
5:N:6:DC:H2'	5:N:7:DT:H71	1.97	0.46
2:D:141:LYS:HA	2:D:141:LYS:HD2	1.60	0.46
3:J:114:VAL:CB	3:J:143:LEU:HD23	2.25	0.46
2:C:297:LEU:CD2	6:O:25:LEU:HD12	2.46	0.46
2:H:229:ASP:OD1	2:I:34:LEU:HD21	2.16	0.46
2:I:15:PHE:HE2	2:I:57:LEU:HB3	1.81	0.46
2:I:101:VAL:HG21	2:I:134:HIS:HB3	1.98	0.45
2:C:246:ASP:O	2:C:247:ASP:C	2.54	0.45
2:G:4:GLN:NE2	2:G:9:LYS:HB2	2.27	0.45
3:J:253:MET:HE2	3:J:290:LEU:CD2	2.45	0.45
3:J:76:TYR:CD1	3:J:111:VAL:HG23	2.51	0.45
2:I:142:THR:O	2:I:146:PRO:HG3	2.15	0.45
2:D:56:ARG:HD3	2:D:92:GLU:OE1	2.16	0.45
2:G:285:MET:O	2:G:288:LEU:HB2	2.16	0.45
2:G:91:ILE:HG22	2:G:93:ILE:CD1	2.45	0.45
2:D:38:HIS:CD2	2:D:39:HIS:H	2.34	0.45
2:D:41:TYR:HB2	2:D:153:LEU:CD2	2.46	0.45
2:C:53:SER:OG	7:C:402:ADP:O1A	2.34	0.45
2:C:326:GLN:HB3	6:O:17:TRP:HB2	1.97	0.45
2:G:294:MET:HA	2:G:297:LEU:HD13	1.98	0.45
3:J:172:ALA:HB1	3:J:191:LEU:CD1	2.46	0.45
2:D:347:MET:O	2:D:351:MET:HG3	2.15	0.45
2:G:292:ILE:HD13	2:G:316:LEU:HD23	1.98	0.45
1:F:170:LEU:HB3	1:F:181:LEU:HD11	1.98	0.45
3:E:90:VAL:HG13	3:E:91:ASP:N	2.31	0.45
2:B:70:ALA:O	2:B:72:PRO:HD2	2.16	0.45
2:D:215:ARG:HH11	3:E:157:SER:HB2	1.81	0.45
2:D:128:VAL:HG13	2:D:162:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:GLN:HG3	1:F:108:LEU:CD2	2.46	0.45
1:A:27:ASP:HA	1:A:28:PRO:HD3	1.68	0.45
2:I:123:TYR:HB2	2:I:152:PHE:CD2	2.51	0.45
2:I:252:LEU:HA	2:I:267:LEU:HD23	1.98	0.45
1:A:296:THR:HG23	1:A:299:ARG:NH1	2.31	0.45
2:I:202:ALA:HB2	2:I:234:THR:HA	1.99	0.45
1:F:4:LEU:HD13	1:F:9:LEU:HA	1.98	0.45
2:B:91:ILE:HG22	2:B:93:ILE:HD13	1.98	0.45
2:G:147:PRO:HB2	2:G:150:VAL:CG2	2.47	0.45
2:I:115:PRO:HD3	2:I:149:HIS:CD2	2.52	0.45
2:H:248:GLN:NE2	2:H:270:GLU:OE2	2.49	0.45
2:C:32:LEU:CD2	2:C:37:ILE:HD11	2.47	0.45
2:I:323:THR:CG2	6:P:8:GLN:OE1	2.64	0.45
2:B:216:ASP:OD1	2:C:168:SER:HB2	2.16	0.45
2:D:101:VAL:HG11	2:D:105:ARG:CZ	2.47	0.45
3:J:46:ARG:HH22	3:J:69:GLN:HE21	1.64	0.45
3:E:68:MET:HA	3:E:68:MET:HE2	1.97	0.45
2:G:46:THR:O	2:G:47:ARG:C	2.54	0.45
3:E:172:ALA:HB1	3:E:191:LEU:CD1	2.45	0.45
2:G:344:ASP:HB3	2:G:347:MET:H	1.81	0.45
2:G:339:LEU:N	2:G:340:PRO:CD	2.80	0.45
3:E:297:ARG:O	3:E:298:GLU:C	2.55	0.45
2:H:291:ARG:HB2	2:H:291:ARG:HE	1.60	0.45
1:F:314:GLN:HB2	3:J:303:VAL:HG22	1.97	0.45
1:F:177:ASN:ND2	1:F:180:ALA:CB	2.80	0.45
1:F:310:LEU:CD2	3:J:306:ILE:CD1	2.95	0.45
3:J:165:ALA:HA	3:J:166:PRO:HD3	1.80	0.45
2:D:221:THR:O	2:D:225:ILE:HG13	2.17	0.45
2:C:95:ALA:O	2:C:99:THR:HG22	2.16	0.45
2:I:101:VAL:HG11	2:I:105:ARG:CZ	2.47	0.45
1:F:42:ALA:C	1:F:47:PHE:HB2	2.37	0.45
3:E:292:ASP:HB3	3:E:315:LEU:HD11	1.99	0.45
2:C:47:ARG:HD3	2:C:47:ARG:H	1.81	0.45
2:H:137:ASN:O	2:H:140:LEU:HB2	2.16	0.45
3:E:197:SER:C	3:E:198:PRO:O	2.55	0.45
2:D:154:LEU:HD23	2:D:154:LEU:HA	1.66	0.45
2:D:221:THR:O	2:D:224:ALA:HB3	2.17	0.45
2:B:92:GLU:HG3	2:B:124:LEU:HG	1.98	0.45
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.76	0.45
1:F:73:LEU:HD12	1:F:73:LEU:N	2.32	0.45
2:B:101:VAL:HG21	2:B:134:HIS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:HIS:CD2	2:I:39:HIS:H	2.34	0.45
2:H:250:LEU:O	2:H:254:GLU:HG3	2.17	0.45
2:B:296:GLN:C	2:B:297:LEU:HD12	2.37	0.45
2:I:32:LEU:HD23	2:I:37:ILE:HD11	1.97	0.45
2:D:60:LYS:HA	2:D:82:ILE:HD12	1.99	0.45
2:D:279:GLU:O	2:D:283:VAL:HG23	2.16	0.45
1:A:251:GLN:NE2	3:E:307:ASN:HD21	2.14	0.45
1:F:6:PRO:HG2	1:F:30:LEU:HD13	1.99	0.45
2:B:311:LEU:HD12	2:B:311:LEU:HA	1.82	0.45
2:D:306:MET:O	2:D:307:ALA:C	2.55	0.45
2:G:158:ASP:OD2	2:G:161:LYS:HE2	2.17	0.45
2:C:144:GLU:HG2	2:C:145:GLU:HG3	1.99	0.45
1:F:29:LEU:HD22	1:F:179:LEU:HA	1.98	0.45
2:G:325:ILE:O	2:G:326:GLN:C	2.55	0.45
1:A:258:VAL:HA	1:A:298:LEU:HD13	1.98	0.45
2:B:306:MET:O	2:B:308:ALA:N	2.50	0.45
2:C:20:GLY:O	2:C:21:GLN:HB2	2.17	0.45
2:H:261:GLY:HA3	2:I:297:LEU:HD11	1.98	0.45
1:F:29:LEU:HD23	1:F:178:LEU:HB3	1.98	0.45
3:J:257:LYS:HB3	3:J:262:ALA:HB3	1.98	0.45
2:C:124:LEU:HA	2:C:153:LEU:O	2.17	0.45
2:G:253:VAL:HG12	2:G:316:LEU:HD21	1.98	0.45
2:H:44:SER:HB3	2:H:159:PRO:HG3	1.99	0.45
1:F:292:ARG:NH1	1:F:293:LEU:HD21	2.32	0.45
3:J:270:VAL:O	3:J:270:VAL:HG23	2.17	0.45
6:O:2:THR:O	6:O:2:THR:HG22	2.16	0.45
2:D:356:ALA:O	2:D:359:PHE:HD2	1.99	0.45
1:F:97:LEU:HD12	1:F:126:TRP:CZ2	2.52	0.44
2:G:78:ASN:O	2:G:82:ILE:HG13	2.16	0.44
2:C:47:ARG:NH2	2:C:211:GLU:O	2.50	0.44
2:B:215:ARG:O	2:B:216:ASP:C	2.55	0.44
3:J:121:THR:CG2	3:J:122:ASP:H	2.27	0.44
2:C:339:LEU:HD11	2:C:345:ARG:O	2.16	0.44
2:D:291:ARG:O	2:D:294:MET:N	2.50	0.44
2:H:326:GLN:HB3	6:P:17:TRP:HB2	1.98	0.44
2:D:257:VAL:HG12	2:D:328:TYR:CE2	2.52	0.44
2:B:112:GLN:OE1	2:B:112:GLN:HA	2.17	0.44
2:I:141:LYS:HD2	2:I:141:LYS:HA	1.53	0.44
2:D:215:ARG:NE	7:D:404:ADP:H5'1	2.33	0.44
2:D:128:VAL:C	2:D:130:MET:N	2.71	0.44
2:I:295:VAL:CG2	2:I:302:LEU:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:C	2:B:42:LEU:HD12	2.38	0.44
1:F:27:ASP:O	1:F:31:LEU:HG	2.18	0.44
5:N:6:DC:H2''	5:N:7:DT:O5'	2.17	0.44
2:H:140:LEU:HD23	2:H:140:LEU:HA	1.81	0.44
2:C:130:MET:CE	2:D:134:HIS:CD2	3.00	0.44
2:C:339:LEU:HB3	2:C:340:PRO:HD3	2.00	0.44
2:H:339:LEU:HD11	2:H:345:ARG:O	2.18	0.44
1:A:170:LEU:HB3	1:A:181:LEU:HD11	1.99	0.44
2:C:37:ILE:HG22	2:C:38:HIS:O	2.17	0.44
2:B:247:ASP:O	2:B:249:ALA:N	2.50	0.44
5:L:4:DG:H2''	5:L:5:DC:O5'	2.17	0.44
3:E:135:PRO:O	3:E:136:PRO:O	2.35	0.44
3:J:147:GLU:HG3	3:J:147:GLU:O	2.16	0.44
1:A:13:LEU:HD13	1:A:38:VAL:HG22	1.99	0.44
2:G:291:ARG:CG	2:G:306:MET:HE3	2.38	0.44
2:C:309:ILE:CG2	2:C:313:MET:HG2	2.47	0.44
1:F:52:THR:CG2	1:F:81:LEU:HD23	2.47	0.44
1:A:233:LEU:O	1:A:234:GLN:C	2.56	0.44
2:B:332:LEU:HD23	2:B:352:THR:CG2	2.47	0.44
2:G:70:ALA:O	2:G:72:PRO:HD2	2.18	0.44
3:J:300:LEU:HD23	3:J:300:LEU:HA	1.66	0.44
2:G:205:LEU:HD23	2:G:205:LEU:HA	1.87	0.44
2:H:294:MET:O	2:H:297:LEU:N	2.50	0.44
3:E:285:ARG:O	3:E:286:LEU:C	2.55	0.44
2:C:101:VAL:HG23	4:K:12:DC:H5''	1.99	0.44
2:I:21:GLN:HE22	2:I:49:VAL:CG1	2.30	0.44
2:B:309:ILE:HG22	2:B:313:MET:CG	2.47	0.44
3:J:176:LEU:HA	3:J:176:LEU:HD23	1.76	0.44
2:D:355:ARG:NE	3:E:332:PRO:HD2	2.32	0.44
2:I:140:LEU:HA	2:I:140:LEU:HD23	1.66	0.44
2:B:101:VAL:O	2:B:102:GLU:C	2.55	0.44
2:H:316:LEU:HD23	2:H:320:ILE:HD11	1.99	0.44
2:G:91:ILE:HG22	2:G:93:ILE:HD13	1.99	0.44
1:F:162:LEU:HD23	1:F:162:LEU:HA	1.68	0.44
2:C:51:LYS:N	7:C:402:ADP:O2B	2.51	0.44
3:J:10:ASP:OD2	3:J:164:LEU:HD12	2.17	0.44
1:F:26:ASN:OD1	1:F:27:ASP:N	2.51	0.44
3:J:151:LEU:HA	3:J:151:LEU:HD12	1.77	0.44
2:I:221:THR:O	2:I:224:ALA:HB3	2.18	0.44
2:D:25:LEU:HD21	2:D:54:ILE:HD13	2.00	0.44
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:116:ASP:HA	3:J:144:ALA:O	2.17	0.44
2:C:318:ARG:NH1	2:C:318:ARG:CB	2.67	0.44
1:F:73:LEU:HD12	1:F:73:LEU:H	1.82	0.44
2:B:50:GLY:O	2:B:51:LYS:C	2.55	0.44
2:C:158:ASP:HA	2:C:159:PRO:HD3	1.59	0.44
2:I:297:LEU:HA	2:I:297:LEU:HD12	1.79	0.44
3:E:224:VAL:CB	3:E:225:PRO:HD3	2.42	0.44
3:E:81:PRO:HB3	3:E:87:THR:O	2.16	0.44
2:B:10:TRP:NE1	2:B:190:ILE:HG23	2.32	0.44
1:A:143:GLU:O	1:A:145:ALA:N	2.50	0.44
2:G:261:GLY:HA3	2:H:297:LEU:HD11	2.00	0.44
2:C:359:PHE:CZ	2:D:323:THR:HG23	2.52	0.44
2:G:179:ASP:OD1	2:G:180:VAL:N	2.51	0.44
2:I:26:THR:HG22	2:I:27:ALA:N	2.33	0.44
2:D:101:VAL:HG21	2:D:134:HIS:HB3	1.99	0.44
2:H:268:ILE:HD11	2:H:353:LEU:CD1	2.45	0.44
2:D:125:ILE:CD1	2:D:125:ILE:H	2.31	0.44
2:G:46:THR:HG22	2:G:47:ARG:HD3	2.00	0.44
3:E:76:TYR:CD1	3:E:111:VAL:HG23	2.53	0.44
2:I:292:ILE:HG22	2:I:325:ILE:HD13	1.99	0.44
1:A:244:VAL:HG21	4:K:5:DT:C5	2.52	0.44
1:F:310:LEU:HD23	3:J:306:ILE:HD12	1.99	0.44
2:C:265:MET:CE	2:C:350:GLU:HG2	2.48	0.44
2:B:11:ARG:HA	2:B:12:PRO:HD3	1.79	0.44
1:F:258:VAL:HA	1:F:298:LEU:HD13	1.98	0.44
2:I:143:LEU:HD12	2:I:143:LEU:HA	1.82	0.44
2:H:166:ILE:HD13	2:H:166:ILE:HA	1.83	0.44
1:A:94:ASN:OD1	1:A:126:TRP:CZ2	2.71	0.44
3:J:286:LEU:HA	3:J:286:LEU:HD23	1.81	0.44
1:F:196:LYS:O	1:F:201:ARG:NH1	2.50	0.44
1:A:213:THR:HG23	1:A:216:HIS:CD2	2.53	0.44
2:C:223:GLN:HG3	2:C:240:MET:HE1	1.99	0.44
2:C:265:MET:HG3	2:D:297:LEU:HD23	2.00	0.44
1:F:233:LEU:O	1:F:234:GLN:C	2.55	0.44
1:F:39:ARG:HD3	1:F:50:HIS:ND1	2.33	0.43
2:B:253:VAL:CG1	2:B:316:LEU:HD21	2.47	0.43
1:A:218:VAL:HG23	1:A:219:ASP:N	2.33	0.43
2:B:331:THR:HG23	6:O:17:TRP:HH2	1.78	0.43
2:I:190:ILE:HD12	2:I:218:LEU:HD21	2.00	0.43
2:H:94:ASP:C	2:H:94:ASP:OD1	2.56	0.43
2:G:112:GLN:OE1	2:G:112:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:268:ILE:HD13	2:G:350:GLU:HG2	1.99	0.43
1:A:47:PHE:CE2	1:A:77:ARG:HB3	2.52	0.43
2:G:302:LEU:HD12	2:G:310:GLU:HG3	2.00	0.43
2:G:101:VAL:CG2	2:G:134:HIS:CB	2.94	0.43
2:C:339:LEU:N	2:C:340:PRO:CD	2.78	0.43
2:D:263:ARG:HG3	2:D:263:ARG:O	2.18	0.43
2:C:41:TYR:HB2	2:C:153:LEU:CD2	2.48	0.43
2:D:341:TYR:N	2:D:341:TYR:HD1	2.16	0.43
2:C:206:LEU:HG	2:C:237:VAL:HG11	1.99	0.43
2:G:260:ASN:ND2	2:G:263:ARG:HB2	2.33	0.43
2:G:319:THR:O	2:G:320:ILE:HG13	2.19	0.43
2:B:32:LEU:HD21	2:B:62:LEU:HD23	2.00	0.43
1:A:147:LEU:O	1:A:148:PRO:C	2.54	0.43
2:G:10:TRP:NE1	2:G:190:ILE:HG23	2.32	0.43
1:F:316:TYR:CE2	5:N:10:DA:C2	3.06	0.43
2:G:8:ARG:NH1	2:H:146:PRO:HD2	2.34	0.43
3:J:232:LEU:O	3:J:233:LEU:C	2.57	0.43
2:H:130:MET:HE3	2:I:134:HIS:CD2	2.53	0.43
2:I:353:LEU:HA	2:I:353:LEU:HD23	1.76	0.43
1:F:47:PHE:CE2	1:F:77:ARG:HB3	2.52	0.43
2:H:215:ARG:O	2:H:216:ASP:C	2.56	0.43
1:F:190:LEU:HD21	2:G:36:ARG:CD	2.45	0.43
2:B:46:THR:O	2:B:47:ARG:C	2.55	0.43
2:I:342:ALA:HA	2:I:343:PRO:HD3	1.86	0.43
2:B:339:LEU:N	2:B:340:PRO:CD	2.82	0.43
2:G:41:TYR:CD1	2:G:41:TYR:N	2.86	0.43
2:C:215:ARG:O	2:C:216:ASP:C	2.57	0.43
2:H:265:MET:HG3	2:I:297:LEU:HD23	2.01	0.43
2:D:123:TYR:HB2	2:D:152:PHE:CD2	2.53	0.43
1:A:28:PRO:CB	2:B:164:VAL:HG21	2.45	0.43
1:A:223:MET:CG	1:A:285:MET:HG3	2.48	0.43
3:J:246:HIS:O	3:J:250:THR:HG23	2.19	0.43
2:H:57:LEU:HA	2:H:57:LEU:HD23	1.80	0.43
2:G:357:LEU:O	6:P:21:ARG:HD2	2.19	0.43
3:J:207:GLY:C	3:J:209:ASN:N	2.70	0.43
2:C:32:LEU:HD23	2:C:37:ILE:HD11	2.01	0.43
3:E:329:LEU:HA	3:E:330:PRO:HD3	1.89	0.43
1:F:254:LEU:HA	1:F:254:LEU:HD12	1.69	0.43
2:G:288:LEU:HD23	2:G:288:LEU:HA	1.68	0.43
3:E:155:LEU:HD12	3:E:155:LEU:C	2.39	0.43
3:E:286:LEU:HA	3:E:286:LEU:HD23	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:GLU:C	2:C:340:PRO:HD2	2.38	0.43
2:B:341:TYR:CZ	2:C:337:LYS:HG3	2.54	0.43
2:D:277:GLU:HG2	2:D:280:ALA:H	1.84	0.43
2:H:224:ALA:HA	2:H:240:MET:CE	2.49	0.43
2:C:74:GLY:HA2	2:C:79:CYS:HB3	2.01	0.43
1:F:55:ILE:HG22	1:F:93:ILE:HD13	2.00	0.43
2:G:302:LEU:HA	2:G:302:LEU:HD23	1.57	0.43
4:K:10:DG:H2''	4:K:11:DG:O5'	2.19	0.43
2:H:327:LEU:O	2:H:327:LEU:HD12	2.19	0.43
2:I:309:ILE:O	2:I:312:ARG:N	2.50	0.43
2:B:49:VAL:CG1	2:B:49:VAL:O	2.66	0.43
2:I:41:TYR:HB2	2:I:153:LEU:HD22	2.00	0.43
2:B:47:ARG:NH2	2:B:211:GLU:O	2.51	0.43
2:G:223:GLN:HB2	2:H:171:LEU:HD22	2.01	0.43
1:F:306:THR:HG23	3:J:311:LEU:CD1	2.48	0.43
1:A:273:PHE:HB3	1:A:283:ARG:HD2	2.00	0.43
1:F:310:LEU:HA	1:F:310:LEU:HD23	1.84	0.43
1:F:68:CYS:SG	1:F:100:LEU:HD23	2.59	0.43
3:E:14:LEU:HD21	3:E:162:HIS:ND1	2.33	0.43
3:E:319:ILE:O	3:E:322:TYR:HB2	2.19	0.43
2:H:299:PRO:HD2	2:H:300:ALA:H	1.83	0.43
1:A:94:ASN:OD1	1:A:126:TRP:NE1	2.51	0.43
2:G:306:MET:O	2:G:308:ALA:N	2.52	0.43
3:E:277:LEU:HD23	3:E:281:LEU:HD13	2.00	0.43
3:J:297:ARG:O	3:J:298:GLU:C	2.55	0.43
2:G:44:SER:HA	2:G:156:THR:O	2.19	0.43
2:G:338:GLU:C	2:G:340:PRO:CD	2.87	0.43
2:C:34:LEU:HD23	2:C:34:LEU:HA	1.75	0.43
1:A:319:SER:HB2	1:A:323:GLU:OE2	2.18	0.43
3:E:249:ALA:HB2	3:E:293:VAL:CG1	2.49	0.43
2:G:107:LEU:HG	2:G:107:LEU:O	2.16	0.43
2:C:297:LEU:HD13	2:C:297:LEU:C	2.39	0.43
2:B:87:PHE:O	2:B:88:VAL:C	2.57	0.43
1:F:147:LEU:O	1:F:148:PRO:C	2.56	0.43
1:A:305:LEU:HD13	1:A:327:LEU:CD2	2.48	0.43
1:A:177:ASN:ND2	1:A:180:ALA:CB	2.82	0.43
2:I:144:GLU:HB2	2:I:169:ARG:HE	1.84	0.43
2:D:144:GLU:HB2	2:D:169:ARG:HE	1.83	0.43
2:C:24:VAL:HG21	2:C:175:LEU:CD2	2.49	0.43
2:C:47:ARG:HH11	2:D:164:VAL:CG2	2.32	0.43
2:G:216:ASP:OD1	2:H:168:SER:CB	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:MET:HG2	3:E:197:SER:CB	2.49	0.43
2:B:189:HIS:O	2:B:192:ASN:HB2	2.19	0.43
3:J:27:LEU:HD12	3:J:27:LEU:HA	1.89	0.43
2:I:187:LEU:HA	2:I:187:LEU:HD23	1.81	0.43
1:A:215:PHE:HE1	4:K:3:DT:C5	2.37	0.42
2:G:20:GLY:O	2:G:21:GLN:HB2	2.18	0.42
3:E:285:ARG:HD3	3:E:323:LEU:HA	2.01	0.42
1:F:25:GLY:O	1:F:115:ASN:HA	2.19	0.42
2:I:114:ALA:HA	2:I:149:HIS:CD2	2.54	0.42
1:F:174:TYR:HB2	1:F:181:LEU:HD13	2.01	0.42
2:I:144:GLU:HB2	2:I:169:ARG:NE	2.33	0.42
1:F:22:LEU:HD13	1:F:127:PHE:CE1	2.54	0.42
2:H:276:ILE:HD11	2:H:281:LEU:HD22	2.00	0.42
2:H:37:ILE:HG22	2:H:38:HIS:O	2.19	0.42
2:H:244:LEU:H	2:H:244:LEU:CD1	2.11	0.42
1:F:64:ILE:HD12	1:F:96:GLN:CG	2.48	0.42
3:J:100:LEU:HA	3:J:100:LEU:HD23	1.85	0.42
3:J:233:LEU:HD12	3:J:237:ASN:HB2	2.02	0.42
2:I:245:ASP:OD1	2:I:245:ASP:O	2.37	0.42
3:J:4:TYR:CG	3:J:6:TRP:CZ2	3.07	0.42
2:H:216:ASP:OD1	2:I:168:SER:HA	2.19	0.42
2:I:128:VAL:C	2:I:130:MET:N	2.72	0.42
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.43	0.42
2:G:329:TYR:O	2:G:330:GLN:C	2.57	0.42
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.84	0.42
1:F:242:GLU:HB2	1:F:245:ILE:HG13	2.02	0.42
1:F:71:MET:HB2	1:F:105:HIS:CE1	2.54	0.42
2:H:24:VAL:HG21	2:H:175:LEU:CD2	2.50	0.42
2:B:215:ARG:HG2	2:C:168:SER:O	2.18	0.42
2:G:101:VAL:CG2	2:G:134:HIS:HB2	2.49	0.42
2:I:362:ARG:O	2:I:363:MET:CG	2.64	0.42
2:I:104:THR:O	2:I:108:LEU:HG	2.19	0.42
3:E:194:SER:O	3:E:196:GLY:N	2.52	0.42
1:F:247:LEU:CD2	1:F:324:LEU:HD21	2.50	0.42
1:A:22:LEU:HD13	1:A:127:PHE:CE1	2.54	0.42
2:B:101:VAL:CG2	2:B:134:HIS:CB	2.95	0.42
3:E:275:ALA:O	3:E:277:LEU:N	2.53	0.42
1:F:223:MET:CG	1:F:285:MET:HG3	2.50	0.42
3:J:99:LYS:CD	3:J:105:ARG:HH22	2.32	0.42
1:F:174:TYR:O	1:F:175:GLU:C	2.58	0.42
2:I:196:ILE:HD12	2:I:225:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:GLU:HB2	2:D:169:ARG:NE	2.34	0.42
2:G:334:ILE:HG22	2:G:335:GLY:N	2.34	0.42
1:A:262:ARG:HG2	1:A:295:GLN:OE1	2.19	0.42
3:E:8:ARG:N	3:E:9:PRO:CD	2.82	0.42
1:A:4:LEU:HD13	1:A:9:LEU:HA	2.02	0.42
1:A:198:THR:HG23	1:A:201:ARG:HD2	2.02	0.42
1:A:64:ILE:HD12	1:A:96:GLN:CG	2.49	0.42
3:J:285:ARG:HD3	3:J:323:LEU:HA	2.02	0.42
2:C:44:SER:HB3	2:C:159:PRO:HG3	2.01	0.42
2:I:41:TYR:HB2	2:I:153:LEU:CD2	2.49	0.42
2:H:288:LEU:HA	2:H:288:LEU:HD23	1.83	0.42
3:E:31:ALA:HB2	3:E:164:LEU:HB3	2.02	0.42
3:J:199:GLY:HA2	3:J:202:LEU:CB	2.49	0.42
2:C:178:LEU:HD12	2:C:214:LEU:HB2	2.01	0.42
2:C:120:PHE:CE1	2:C:151:LYS:HE2	2.55	0.42
1:F:146:GLN:HG3	1:F:146:GLN:H	1.66	0.42
2:B:235:GLN:HG3	2:B:235:GLN:H	1.64	0.42
2:H:277:GLU:H	2:H:277:GLU:HG3	1.72	0.42
1:A:78:GLN:HG3	1:A:108:LEU:CD2	2.49	0.42
3:J:292:ASP:CG	3:J:318:ARG:HH21	2.23	0.42
3:J:315:LEU:HG	3:J:315:LEU:O	2.19	0.42
2:G:250:LEU:CD2	2:G:312:ARG:NE	2.82	0.42
3:E:222:TYR:CD2	3:E:222:TYR:C	2.93	0.42
2:D:41:TYR:HB2	2:D:153:LEU:HD22	2.02	0.42
2:I:342:ALA:HB1	2:I:343:PRO:HD2	2.00	0.42
2:G:264:VAL:HG21	2:G:357:LEU:HD11	2.01	0.42
3:J:47:TYR:CD2	3:J:48:LEU:HD23	2.54	0.42
3:J:100:LEU:HD11	3:J:112:VAL:HG21	2.02	0.42
2:B:250:LEU:HD23	2:B:312:ARG:NH2	2.34	0.42
2:G:101:VAL:O	2:G:102:GLU:C	2.58	0.42
3:J:121:THR:H	3:J:124:ALA:HB3	1.85	0.42
2:D:250:LEU:HD13	2:D:313:MET:CE	2.49	0.42
1:F:13:LEU:CD1	1:F:38:VAL:HG22	2.48	0.42
3:J:35:MET:HG2	3:J:197:SER:CB	2.50	0.42
3:E:253:MET:HE2	3:E:290:LEU:CD2	2.50	0.42
6:O:21:ARG:N	6:O:22:PRO:HD3	2.35	0.42
2:B:223:GLN:HG2	2:B:240:MET:SD	2.58	0.42
2:B:13:GLN:O	2:B:57:LEU:CD2	2.68	0.42
2:D:356:ALA:HA	2:D:359:PHE:CD2	2.54	0.42
3:J:232:LEU:HB3	3:J:236:LEU:HD11	2.01	0.42
2:I:158:ASP:OD2	2:I:161:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLY:HA2	2:H:79:CYS:HB3	2.01	0.42
2:B:302:LEU:HA	2:B:302:LEU:HD23	1.62	0.42
2:D:327:LEU:HD23	2:D:327:LEU:HA	1.70	0.42
1:F:94:ASN:OD1	1:F:126:TRP:CZ2	2.72	0.42
1:A:9:LEU:HG	1:A:13:LEU:HG	2.02	0.42
2:I:327:LEU:HA	2:I:327:LEU:HD23	1.75	0.42
2:G:250:LEU:HD23	2:G:312:ARG:NE	2.34	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.75	0.42
2:B:294:MET:HA	2:B:297:LEU:HD13	2.01	0.42
2:D:282:LEU:HD23	2:D:282:LEU:HA	1.84	0.42
2:B:248:GLN:H	2:B:248:GLN:CD	2.23	0.42
1:A:42:ALA:O	1:A:47:PHE:CD1	2.73	0.42
1:A:169:VAL:CG2	1:A:199:LEU:HD11	2.50	0.42
2:C:288:LEU:HD22	2:C:313:MET:SD	2.60	0.42
6:O:20:ARG:O	6:O:21:ARG:HG3	2.19	0.42
5:L:6:DC:H2'	5:L:7:DT:H71	2.01	0.42
2:D:158:ASP:OD2	2:D:161:LYS:HE3	2.19	0.42
3:E:13:LYS:HA	3:E:13:LYS:HD2	1.96	0.42
1:A:146:GLN:H	1:A:146:GLN:HG3	1.70	0.42
2:D:140:LEU:HA	2:D:140:LEU:HD23	1.75	0.42
2:I:215:ARG:CG	2:I:215:ARG:NH1	2.83	0.41
2:B:351:MET:HG3	2:C:329:TYR:CZ	2.54	0.41
2:G:14:THR:CG2	2:G:16:ALA:H	2.19	0.41
1:F:94:ASN:OD1	1:F:126:TRP:NE1	2.53	0.41
2:H:204:GLN:O	2:H:208:ARG:HG3	2.20	0.41
2:H:140:LEU:HD21	2:H:165:THR:HB	2.02	0.41
2:H:265:MET:CE	2:H:350:GLU:HG2	2.50	0.41
2:C:341:TYR:CE2	2:D:337:LYS:HG3	2.55	0.41
2:B:49:VAL:O	2:B:49:VAL:HG12	2.20	0.41
2:C:279:GLU:O	2:C:283:VAL:HG23	2.20	0.41
2:G:292:ILE:HD11	2:G:316:LEU:HD23	2.02	0.41
3:E:112:VAL:HB	3:E:141:PHE:CE1	2.55	0.41
2:C:316:LEU:O	2:C:320:ILE:HG13	2.20	0.41
2:I:43:PHE:N	2:I:154:LEU:O	2.42	0.41
1:A:177:ASN:ND2	1:A:180:ALA:HB2	2.34	0.41
3:E:165:ALA:HA	3:E:166:PRO:HD3	1.80	0.41
2:C:276:ILE:HD11	2:C:281:LEU:HD22	2.01	0.41
3:J:249:ALA:HB2	3:J:293:VAL:HG11	2.01	0.41
2:I:244:LEU:HD11	2:I:281:LEU:HA	2.01	0.41
2:G:232:VAL:O	2:G:232:VAL:HG12	2.20	0.41
2:C:154:LEU:N	2:C:154:LEU:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:LYS:HD3	2:C:194:GLU:OE2	2.20	0.41
4:M:2:DT:H2'	4:M:2:DT:H6	1.70	0.41
1:A:4:LEU:HD13	1:A:9:LEU:HD12	2.03	0.41
2:I:8:ARG:CZ	3:J:135:PRO:HD2	2.51	0.41
2:G:128:VAL:O	2:G:128:VAL:CG2	2.67	0.41
2:I:292:ILE:HD13	2:I:316:LEU:HB3	2.00	0.41
3:J:152:LEU:HD12	3:J:153:ALA:N	2.35	0.41
2:I:354:LEU:O	2:I:355:ARG:C	2.58	0.41
2:D:248:GLN:OE1	2:D:276:ILE:HD11	2.20	0.41
1:F:124:ALA:O	1:F:125:ALA:C	2.57	0.41
3:E:100:LEU:HA	3:E:100:LEU:HD23	1.88	0.41
1:A:73:LEU:HD11	1:A:105:HIS:CD2	2.55	0.41
1:A:81:LEU:HD12	1:A:82:LEU:N	2.35	0.41
1:F:20:ALA:CB	1:F:110:LEU:HD23	2.50	0.41
3:J:285:ARG:HD3	3:J:322:TYR:O	2.20	0.41
2:C:309:ILE:HG22	2:C:313:MET:CG	2.50	0.41
2:H:288:LEU:HD22	2:H:313:MET:SD	2.60	0.41
2:I:267:LEU:HA	2:I:267:LEU:HD12	1.83	0.41
3:E:152:LEU:HD12	3:E:153:ALA:N	2.35	0.41
1:A:318:GLN:O	1:A:319:SER:C	2.59	0.41
3:E:176:LEU:HA	3:E:176:LEU:HD23	1.68	0.41
2:G:5:VAL:HG12	2:G:7:ALA:H	1.86	0.41
2:H:92:GLU:HG3	2:H:124:LEU:HG	2.02	0.41
2:H:206:LEU:HG	2:H:237:VAL:HG11	2.01	0.41
2:B:245:ASP:HB3	2:B:247:ASP:HB2	2.02	0.41
3:J:188:LEU:HD12	3:J:188:LEU:O	2.20	0.41
2:G:191:LEU:HD23	2:G:191:LEU:HA	1.78	0.41
1:F:42:ALA:O	1:F:47:PHE:CD1	2.74	0.41
2:G:215:ARG:NH2	2:H:169:ARG:CZ	2.84	0.41
2:I:250:LEU:HD13	2:I:313:MET:CE	2.51	0.41
2:D:125:ILE:HG21	2:D:131:LEU:HD11	2.03	0.41
1:A:26:ASN:C	1:A:26:ASN:OD1	2.59	0.41
1:A:219:ASP:OD1	1:A:285:MET:HE1	2.20	0.41
2:C:278:TRP:O	2:C:279:GLU:C	2.58	0.41
3:J:20:ALA:HB3	3:J:22:ARG:HG3	2.01	0.41
2:H:15:PHE:HE1	2:H:57:LEU:HB3	1.84	0.41
2:G:343:PRO:HG3	2:H:286:LEU:HB3	2.02	0.41
2:G:347:MET:HE1	2:H:291:ARG:HH21	1.85	0.41
3:J:176:LEU:HD11	3:J:201:ALA:CB	2.51	0.41
2:I:166:ILE:HA	2:I:166:ILE:HD13	1.93	0.41
2:B:303:GLY:H	2:B:306:MET:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:CD1	1:A:111:ILE:HG22	2.51	0.41
2:G:291:ARG:O	2:G:295:VAL:HG23	2.21	0.41
1:A:63:ALA:O	1:A:67:LEU:HG	2.20	0.41
1:F:53:PHE:CZ	1:F:67:LEU:HD11	2.55	0.41
2:H:320:ILE:HG22	2:H:321:PRO:HD2	2.01	0.41
2:I:343:PRO:HB3	3:J:246:HIS:ND1	2.34	0.41
2:H:309:ILE:CG2	2:H:313:MET:HG2	2.50	0.41
2:G:42:LEU:HA	2:G:154:LEU:O	2.20	0.41
2:D:10:TRP:NE1	2:D:190:ILE:HG23	2.34	0.41
1:F:56:ASP:CB	1:F:58:ASN:H	2.33	0.41
1:F:68:CYS:SG	1:F:100:LEU:CD2	3.09	0.41
3:J:128:LEU:O	3:J:132:LEU:HB2	2.20	0.41
2:I:25:LEU:HD21	2:I:54:ILE:HD13	2.02	0.41
2:H:47:ARG:NH2	2:H:211:GLU:O	2.54	0.41
3:J:292:ASP:HB3	3:J:315:LEU:HD11	2.01	0.41
2:B:82:ILE:HG23	2:B:90:LEU:CD2	2.39	0.41
2:D:309:ILE:O	2:D:312:ARG:N	2.46	0.41
1:A:158:LEU:O	1:A:160:LEU:HG	2.20	0.41
2:B:121:LYS:N	2:B:149:HIS:O	2.53	0.41
2:H:278:TRP:HE1	2:H:346:ARG:HB2	1.82	0.41
2:H:250:LEU:HD13	2:H:288:LEU:HD13	2.03	0.41
2:B:57:LEU:HD23	2:B:57:LEU:HA	1.65	0.41
2:G:160:GLN:HG3	2:G:160:GLN:O	2.21	0.41
2:H:6:LEU:HA	2:H:6:LEU:HD23	1.90	0.41
1:F:97:LEU:CD1	1:F:126:TRP:CH2	3.03	0.41
1:A:18:ARG:HD3	1:A:133:ARG:O	2.21	0.41
2:H:137:ASN:H	2:H:137:ASN:ND2	2.17	0.41
2:C:353:LEU:O	2:C:357:LEU:HG	2.20	0.41
2:B:101:VAL:CG2	2:B:134:HIS:HB2	2.51	0.41
2:G:91:ILE:HD13	2:G:123:TYR:CE2	2.55	0.41
2:C:5:VAL:HG12	2:C:5:VAL:O	2.16	0.41
2:B:282:LEU:HD21	2:B:349:VAL:HG13	2.03	0.41
3:J:216:LEU:HD12	3:J:216:LEU:HA	1.83	0.41
2:D:111:VAL:O	2:D:113:TYR:N	2.54	0.41
2:C:44:SER:HA	2:C:156:THR:O	2.21	0.41
2:G:294:MET:C	2:G:296:GLN:N	2.73	0.41
2:D:104:THR:O	2:D:108:LEU:HG	2.21	0.41
2:B:332:LEU:HD23	2:B:352:THR:HG21	2.02	0.41
2:I:276:ILE:HG21	2:I:281:LEU:HD13	2.03	0.41
2:B:205:LEU:HA	2:B:205:LEU:HD23	1.85	0.41
2:I:111:VAL:HG13	2:I:150:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:27:GLY:O	6:P:28:GLU:C	2.59	0.41
1:F:47:PHE:CD2	1:F:77:ARG:HB3	2.56	0.41
1:A:13:LEU:HD22	1:A:21:TYR:CZ	2.55	0.41
2:I:128:VAL:HG13	2:I:162:LEU:HD21	2.03	0.41
1:A:90:ASN:O	1:A:94:ASN:HB2	2.20	0.41
7:G:406:ADP:N3	7:G:406:ADP:H2'	2.36	0.41
3:J:224:VAL:HG12	3:J:225:PRO:N	2.34	0.41
2:B:20:GLY:HA2	2:B:22:GLU:OE2	2.21	0.41
2:H:11:ARG:HG3	2:H:53:SER:CB	2.47	0.41
2:G:341:TYR:CE1	2:H:337:LYS:HE3	2.56	0.41
2:C:282:LEU:HG	2:C:349:VAL:HG22	2.02	0.41
3:E:275:ALA:O	3:E:278:ALA:N	2.53	0.41
2:I:252:LEU:HD13	2:I:285:MET:HE2	2.03	0.41
6:P:21:ARG:N	6:P:22:PRO:HD3	2.36	0.41
3:E:99:LYS:CD	3:E:105:ARG:HH22	2.34	0.41
2:C:32:LEU:HA	2:C:32:LEU:HD23	1.86	0.41
2:D:244:LEU:HD11	2:D:281:LEU:HA	2.03	0.41
2:D:11:ARG:O	2:D:13:GLN:HG2	2.21	0.41
2:I:214:LEU:HA	2:I:214:LEU:HD23	1.83	0.41
2:G:162:LEU:HA	2:G:163:PRO:HD3	1.94	0.41
2:D:203:LEU:HD23	2:D:203:LEU:HA	1.72	0.41
3:J:13:LYS:HD2	3:J:13:LYS:HA	1.87	0.41
2:C:140:LEU:HD21	2:C:165:THR:HB	2.03	0.41
3:E:103:HIS:H	3:E:103:HIS:HD2	1.65	0.41
3:E:275:ALA:O	3:E:276:GLU:C	2.58	0.41
2:D:107:LEU:HD22	2:D:107:LEU:HA	1.80	0.41
3:J:242:PRO:O	3:J:297:ARG:HD2	2.21	0.41
2:D:347:MET:HE1	3:E:250:THR:HG22	2.02	0.41
2:I:248:GLN:OE1	2:I:276:ILE:HD11	2.21	0.41
1:F:255:LEU:HD22	3:J:313:THR:HG21	2.02	0.41
2:I:52:THR:OG1	2:I:126:ASP:OD1	2.39	0.41
3:E:282:SER:HB2	3:J:279:ASN:O	2.20	0.41
1:F:54:SER:HA	1:F:83:LEU:HB2	2.02	0.41
2:I:258:GLU:O	2:I:259:ALA:HB3	2.19	0.41
3:E:133:GLU:HG2	3:E:134:GLU:HG2	2.02	0.41
2:D:258:GLU:O	2:D:259:ALA:HB3	2.21	0.41
2:G:311:LEU:HA	2:G:311:LEU:HD12	1.80	0.41
2:I:181:GLU:HA	2:I:181:GLU:OE1	2.21	0.41
1:A:81:LEU:HD12	1:A:82:LEU:H	1.86	0.40
1:A:47:PHE:CD2	1:A:77:ARG:HB3	2.56	0.40
3:J:155:LEU:C	3:J:155:LEU:HD12	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:H	1:A:117:LEU:HG	1.65	0.40
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.81	0.40
2:C:60:LYS:HA	2:C:82:ILE:CD1	2.50	0.40
3:E:135:PRO:C	3:E:136:PRO:O	2.59	0.40
2:C:358:ALA:HA	2:C:365:LEU:HB2	2.02	0.40
2:C:241:LEU:HA	2:C:241:LEU:HD23	1.91	0.40
3:J:46:ARG:HH12	3:J:69:GLN:CG	2.32	0.40
3:E:242:PRO:O	3:E:297:ARG:HD2	2.21	0.40
2:H:358:ALA:HA	2:H:365:LEU:HB2	2.02	0.40
2:H:9:LYS:HD3	2:H:194:GLU:OE2	2.21	0.40
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.67	0.40
2:D:12:PRO:HG3	7:D:404:ADP:C2	2.57	0.40
2:H:47:ARG:NH1	2:H:216:ASP:OD2	2.54	0.40
1:F:90:ASN:O	1:F:94:ASN:HB2	2.21	0.40
1:A:55:ILE:HG22	1:A:93:ILE:HD13	2.03	0.40
1:A:204:GLN:O	2:B:176:LYS:HE3	2.22	0.40
2:D:115:PRO:HD3	2:D:149:HIS:CD2	2.57	0.40
1:F:262:ARG:HH22	3:J:320:GLU:CD	2.25	0.40
2:C:277:GLU:O	2:C:280:ALA:HB3	2.22	0.40
3:E:116:ASP:HA	3:E:144:ALA:O	2.21	0.40
1:A:9:LEU:O	1:A:13:LEU:HG	2.21	0.40
2:C:282:LEU:HD23	2:C:282:LEU:HA	1.85	0.40
3:E:198:PRO:O	3:E:200:ALA:N	2.52	0.40
2:I:42:LEU:HD12	2:I:154:LEU:O	2.21	0.40
1:A:6:PRO:HG2	1:A:30:LEU:HD22	2.03	0.40
2:I:279:GLU:O	2:I:283:VAL:HG23	2.22	0.40
2:C:359:PHE:O	2:C:360:HIS:C	2.59	0.40
2:G:303:GLY:H	2:G:306:MET:HG3	1.87	0.40
1:F:63:ALA:O	1:F:67:LEU:HG	2.21	0.40
2:C:162:LEU:HA	2:C:163:PRO:HD3	1.99	0.40
2:C:140:LEU:HD22	2:C:169:ARG:CZ	2.52	0.40
1:F:305:LEU:HA	1:F:305:LEU:HD12	1.74	0.40
1:A:326:GLY:O	1:A:327:LEU:C	2.59	0.40
3:E:76:TYR:CD1	3:E:111:VAL:CG2	3.02	0.40
2:G:87:PHE:O	2:G:88:VAL:C	2.60	0.40
2:D:119:ARG:HG2	2:D:120:PHE:CD2	2.57	0.40
1:F:242:GLU:HA	1:F:243:PRO:HD3	1.97	0.40
1:A:22:LEU:HD23	1:A:112:VAL:HB	2.04	0.40
2:D:289:LEU:HD23	2:D:289:LEU:HA	1.79	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.03	0.17
2:D:88:VAL:CG2	2:G:88:VAL:CG2[2_555]	2.05	0.15
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	331/343 (96%)	293 (88%)	29 (9%)	9 (3%)	6	44
1	F	332/343 (97%)	295 (89%)	30 (9%)	7 (2%)	9	50
2	B	357/395 (90%)	314 (88%)	37 (10%)	6 (2%)	11	54
2	C	363/395 (92%)	317 (87%)	42 (12%)	4 (1%)	17	63
2	D	360/395 (91%)	310 (86%)	40 (11%)	10 (3%)	6	43
2	G	371/395 (94%)	334 (90%)	30 (8%)	7 (2%)	10	51
2	H	363/395 (92%)	315 (87%)	43 (12%)	5 (1%)	14	58
2	I	360/395 (91%)	315 (88%)	38 (11%)	7 (2%)	10	51
3	E	332/334 (99%)	299 (90%)	28 (8%)	5 (2%)	13	56
3	J	332/334 (99%)	299 (90%)	29 (9%)	4 (1%)	16	61
6	O	25/27 (93%)	20 (80%)	1 (4%)	4 (16%)	0	3
6	P	25/27 (93%)	20 (80%)	2 (8%)	3 (12%)	0	6
All	All	3551/3778 (94%)	3131 (88%)	349 (10%)	71 (2%)	9	51

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	159	ASN
1	A	320	VAL
2	B	247	ASP
2	B	248	GLN

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Mol	Chain	Res	Type
2	B	305	ASP
2	B	306	MET
2	B	307	ALA
2	D	116	ALA
1	F	60	ASP
1	F	159	ASN
1	F	320	VAL
2	G	247	ASP
2	G	248	GLN
2	G	305	ASP
2	G	306	MET
2	G	307	ALA
2	I	116	ALA
6	O	26	GLN
6	O	27	GLY
6	P	26	GLN
6	P	27	GLY
1	A	144	GLN
2	C	195	HIS
2	D	338	GLU
3	E	71	GLY
2	H	195	HIS
6	O	20	ARG
6	P	20	ARG
1	A	125	ALA
2	B	47	ARG
2	C	308	ALA
2	D	307	ALA
2	D	310	GLU
2	D	337	LYS
3	E	82	GLU
1	F	125	ALA
1	F	131	ALA
2	G	47	ARG
2	H	308	ALA
2	I	132	SER
2	I	307	ALA
2	I	310	GLU
3	J	71	GLY
1	A	131	ALA
2	C	356	ALA
2	C	364	PRO

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Mol	Chain	Res	Type
2	D	51	LYS
2	D	132	SER
3	E	136	PRO
1	F	144	GLN
2	I	188	GLU
2	I	337	LYS
2	I	338	GLU
3	J	82	GLU
3	J	136	PRO
1	A	115	ASN
1	A	233	LEU
1	A	327	LEU
2	D	188	GLU
1	F	233	LEU
2	H	110	ASN
2	H	356	ALA
6	O	19	LEU
2	D	323	THR
2	H	364	PRO
3	J	268	VAL
3	E	268	VAL
2	G	343	PRO
2	D	322	PRO
3	E	9	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	283/291 (97%)	271 (96%)	12 (4%)	36	74
1	F	284/291 (98%)	271 (95%)	13 (5%)	33	72
2	B	296/329 (90%)	280 (95%)	16 (5%)	27	67
2	C	302/329 (92%)	280 (93%)	22 (7%)	17	57
2	D	299/329 (91%)	286 (96%)	13 (4%)	35	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	308/329 (94%)	290 (94%)	18 (6%)	25	65
2	H	302/329 (92%)	281 (93%)	21 (7%)	19	59
2	I	299/329 (91%)	286 (96%)	13 (4%)	35	74
3	E	270/270 (100%)	255 (94%)	15 (6%)	26	66
3	J	270/270 (100%)	253 (94%)	17 (6%)	22	63
6	O	23/23 (100%)	22 (96%)	1 (4%)	35	74
6	P	23/23 (100%)	22 (96%)	1 (4%)	35	74
All	All	2959/3142 (94%)	2797 (94%)	162 (6%)	27	67

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	73	LEU
1	A	78	GLN
1	A	108	LEU
1	A	117	LEU
1	A	157	GLN
1	A	162	LEU
1	A	163	ASP
1	A	173	CYS
1	A	202	VAL
1	A	207	ASN
1	A	319	SER
2	B	6	LEU
2	B	33	SER
2	B	46	THR
2	B	47	ARG
2	B	93	ILE
2	B	135	SER
2	B	137	ASN
2	B	164	VAL
2	B	216	ASP
2	B	219	SER
2	B	251	SER
2	B	302	LEU
2	B	324	ASP
2	B	325	ILE
2	B	351	MET
2	B	355	ARG

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Mol	Chain	Res	Type
2	C	8	ARG
2	C	46	THR
2	C	47	ARG
2	C	53	SER
2	C	75	VAL
2	C	97	SER
2	C	124	LEU
2	C	137	ASN
2	C	165	THR
2	C	175	LEU
2	C	179	ASP
2	C	214	LEU
2	C	238	SER
2	C	244	LEU
2	C	248	GLN
2	C	252	LEU
2	C	277	GLU
2	C	291	ARG
2	C	299	PRO
2	C	311	LEU
2	C	334	ILE
2	C	365	LEU
2	D	6	LEU
2	D	30	ASN
2	D	47	ARG
2	D	54	ILE
2	D	104	THR
2	D	107	LEU
2	D	117	ARG
2	D	157	THR
2	D	165	THR
2	D	215	ARG
2	D	252	LEU
2	D	305	ASP
2	D	330	GLN
3	E	50	CYS
3	E	68	MET
3	E	145	THR
3	E	154	THR
3	E	155	LEU
3	E	157	SER
3	E	160	ARG

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Mol	Chain	Res	Type
3	E	180	VAL
3	E	181	THR
3	E	202	LEU
3	E	208	ASP
3	E	231	SER
3	E	253	MET
3	E	277	LEU
3	E	304	THR
1	F	64	ILE
1	F	73	LEU
1	F	78	GLN
1	F	108	LEU
1	F	117	LEU
1	F	157	GLN
1	F	162	LEU
1	F	173	CYS
1	F	202	VAL
1	F	207	ASN
1	F	308	THR
1	F	314	GLN
1	F	319	SER
2	G	-7	GLU
2	G	-5	LEU
2	G	6	LEU
2	G	33	SER
2	G	46	THR
2	G	47	ARG
2	G	93	ILE
2	G	135	SER
2	G	137	ASN
2	G	157	THR
2	G	164	VAL
2	G	216	ASP
2	G	251	SER
2	G	302	LEU
2	G	324	ASP
2	G	325	ILE
2	G	351	MET
2	G	355	ARG
2	H	8	ARG
2	H	46	THR
2	H	47	ARG

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Mol	Chain	Res	Type
2	H	53	SER
2	H	75	VAL
2	H	97	SER
2	H	124	LEU
2	H	165	THR
2	H	175	LEU
2	H	179	ASP
2	H	214	LEU
2	H	238	SER
2	H	244	LEU
2	H	248	GLN
2	H	252	LEU
2	H	277	GLU
2	H	291	ARG
2	H	311	LEU
2	H	318	ARG
2	H	334	ILE
2	H	365	LEU
2	I	6	LEU
2	I	30	ASN
2	I	47	ARG
2	I	54	ILE
2	I	104	THR
2	I	107	LEU
2	I	117	ARG
2	I	157	THR
2	I	165	THR
2	I	215	ARG
2	I	252	LEU
2	I	305	ASP
2	I	330	GLN
3	J	50	CYS
3	J	68	MET
3	J	145	THR
3	J	154	THR
3	J	155	LEU
3	J	157	SER
3	J	160	ARG
3	J	180	VAL
3	J	181	THR
3	J	202	LEU
3	J	208	ASP

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Mol	Chain	Res	Type
3	J	218	GLN
3	J	231	SER
3	J	253	MET
3	J	277	LEU
3	J	285	ARG
3	J	304	THR
6	O	10	GLN
6	P	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	51	HIS
1	A	105	HIS
1	A	177	ASN
1	A	207	ASN
1	A	216	HIS
1	A	266	HIS
1	A	333	HIS
2	B	39	HIS
2	B	84	GLN
2	B	248	GLN
2	B	260	ASN
2	B	290	HIS
2	C	23	HIS
2	C	112	GLN
2	C	137	ASN
2	C	149	HIS
2	C	290	HIS
2	D	38	HIS
2	D	134	HIS
2	D	172	GLN
2	D	204	GLN
2	D	330	GLN
3	E	30	GLN
3	E	52	GLN
3	E	54	GLN
3	E	56	HIS
3	E	103	HIS
3	E	267	ASN
3	E	307	ASN

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Mol	Chain	Res	Type
1	F	50	HIS
1	F	51	HIS
1	F	105	HIS
1	F	177	ASN
1	F	207	ASN
1	F	216	HIS
1	F	333	HIS
2	G	4	GLN
2	G	39	HIS
2	G	84	GLN
2	G	260	ASN
2	H	23	HIS
2	H	112	GLN
2	H	137	ASN
2	H	290	HIS
2	I	30	ASN
2	I	38	HIS
2	I	134	HIS
2	I	172	GLN
2	I	204	GLN
2	I	330	GLN
3	J	30	GLN
3	J	52	GLN
3	J	54	GLN
3	J	56	HIS
3	J	103	HIS
3	J	260	HIS
3	J	267	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 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
7	ADP	B	400	9,8	22,29,29	1.05	1 (4%)	27,45,45	2.01	6 (22%)
8	BEF	B	401	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	C	402	9,8	22,29,29	1.05	1 (4%)	27,45,45	2.12	6 (22%)
8	BEF	C	403	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	D	404	9,8	22,29,29	1.10	1 (4%)	27,45,45	1.94	6 (22%)
8	BEF	D	405	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	G	406	9,8	22,29,29	1.10	1 (4%)	27,45,45	2.04	7 (25%)
8	BEF	G	407	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	H	408	9,8	22,29,29	1.17	2 (9%)	27,45,45	2.22	5 (18%)
8	BEF	H	409	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	I	410	9,8	22,29,29	1.10	2 (9%)	27,45,45	1.99	6 (22%)
8	BEF	I	411	7	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	B	400	9,8	-	0/12/32/32	0/3/3/3
8	BEF	B	401	7	-	0/0/0/0	0/0/0/0
7	ADP	C	402	9,8	-	0/12/32/32	0/3/3/3
8	BEF	C	403	7	-	0/0/0/0	0/0/0/0
7	ADP	D	404	9,8	-	0/12/32/32	0/3/3/3
8	BEF	D	405	7	-	0/0/0/0	0/0/0/0
7	ADP	G	406	9,8	-	0/12/32/32	0/3/3/3
8	BEF	G	407	7	-	0/0/0/0	0/0/0/0
7	ADP	H	408	9,8	-	0/12/32/32	0/3/3/3
8	BEF	H	409	7	-	0/0/0/0	0/0/0/0
7	ADP	I	410	9,8	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BEF	I	411	7	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	410	ADP	C5-N7	-2.01	1.32	1.39
7	I	410	ADP	C5-C4	2.32	1.45	1.40
7	H	408	ADP	PB-O3B	2.34	1.63	1.54
7	B	400	ADP	C5-C4	2.86	1.47	1.40
7	D	404	ADP	C5-C4	3.03	1.47	1.40
7	H	408	ADP	C5-C4	3.08	1.47	1.40
7	G	406	ADP	C5-C4	3.15	1.47	1.40
7	C	402	ADP	C5-C4	3.16	1.47	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	408	ADP	N3-C2-N1	-6.67	123.79	128.89
7	G	406	ADP	N3-C2-N1	-6.52	123.90	128.89
7	B	400	ADP	N3-C2-N1	-6.33	124.05	128.89
7	C	402	ADP	N3-C2-N1	-6.33	124.05	128.89
7	D	404	ADP	N3-C2-N1	-5.37	124.78	128.89
7	I	410	ADP	N3-C2-N1	-4.84	125.19	128.89
7	H	408	ADP	C2'-C1'-N9	-4.78	106.99	114.29
7	H	408	ADP	PA-O3A-PB	-4.63	117.14	132.67
7	C	402	ADP	PA-O3A-PB	-4.61	117.22	132.67
7	B	400	ADP	C2'-C1'-N9	-4.31	107.71	114.29
7	D	404	ADP	PA-O3A-PB	-4.01	119.24	132.67
7	I	410	ADP	PA-O3A-PB	-3.87	119.68	132.67
7	G	406	ADP	C2'-C1'-N9	-3.85	108.41	114.29
7	C	402	ADP	C2'-C1'-N9	-3.76	108.55	114.29
7	G	406	ADP	PA-O3A-PB	-3.03	122.49	132.67
7	C	402	ADP	C4-C5-N7	-3.00	106.72	109.48
7	B	400	ADP	PA-O3A-PB	-2.87	123.05	132.67
7	I	410	ADP	C2'-C1'-N9	-2.80	110.01	114.29
7	D	404	ADP	C2'-C1'-N9	-2.63	110.28	114.29
7	D	404	ADP	C4-C5-N7	-2.52	107.16	109.48
7	G	406	ADP	C4-C5-N7	-2.42	107.25	109.48
7	B	400	ADP	C4-C5-N7	-2.30	107.36	109.48
7	B	400	ADP	O3B-PB-O2B	-2.02	99.70	107.38
7	H	408	ADP	O3A-PA-O5'	2.14	108.62	102.94
7	G	406	ADP	C2-N1-C6	2.34	122.96	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	402	ADP	C4'-O4'-C1'	2.55	112.52	109.72
7	G	406	ADP	O3A-PA-O5'	2.59	109.80	102.94
7	D	404	ADP	C4'-O4'-C1'	2.71	112.70	109.72
7	I	410	ADP	O3A-PA-O5'	3.08	111.11	102.94
7	G	406	ADP	O2B-PB-O1B	3.35	121.38	110.58
7	B	400	ADP	O2B-PB-O1B	3.57	122.06	110.58
7	H	408	ADP	O2B-PB-O1B	3.60	122.18	110.58
7	C	402	ADP	O2B-PB-O1B	3.61	122.19	110.58
7	D	404	ADP	O2B-PB-O1B	3.85	122.97	110.58
7	I	410	ADP	C4'-O4'-C1'	3.86	113.97	109.72
7	I	410	ADP	O2B-PB-O1B	3.91	123.18	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	400	ADP	4	0
7	C	402	ADP	4	0
7	D	404	ADP	5	0
7	G	406	ADP	5	0
7	H	408	ADP	4	0
7	I	410	ADP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	333/343 (97%)	0.75	39 (11%) 6 6	75, 139, 217, 248	0
1	F	334/343 (97%)	0.80	47 (14%) 4 4	78, 147, 225, 251	0
2	B	359/395 (90%)	0.05	1 (0%) 94 91	81, 116, 159, 175	0
2	C	365/395 (92%)	-0.09	1 (0%) 94 91	76, 116, 166, 198	0
2	D	362/395 (91%)	0.12	2 (0%) 90 85	77, 111, 154, 195	0
2	G	373/395 (94%)	0.07	9 (2%) 62 52	71, 113, 164, 236	0
2	H	365/395 (92%)	-0.21	0 100 100	68, 88, 131, 164	0
2	I	362/395 (91%)	0.00	3 (0%) 87 80	64, 86, 131, 171	0
3	E	334/334 (100%)	0.04	6 (1%) 71 62	71, 92, 164, 216	0
3	J	334/334 (100%)	0.22	7 (2%) 67 58	71, 92, 160, 222	0
4	K	14/15 (93%)	0.38	2 (14%) 4 4	89, 99, 195, 205	0
4	M	14/15 (93%)	0.10	0 100 100	90, 95, 197, 219	0
5	L	10/10 (100%)	-0.43	0 100 100	96, 104, 110, 110	0
5	N	10/10 (100%)	-0.42	0 100 100	88, 97, 117, 119	0
6	O	27/27 (100%)	0.31	1 (3%) 45 36	83, 125, 187, 193	0
6	P	27/27 (100%)	0.15	1 (3%) 45 36	69, 105, 163, 168	0
All	All	3623/3828 (94%)	0.16	119 (3%) 50 41	64, 107, 188, 251	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TRP	7.3
3	J	56	HIS	7.0
1	F	57	PRO	6.5
3	J	55	GLY	6.3
3	J	54	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
2	G	-8	LEU	5.7
1	A	53	PHE	5.5
1	A	128	THR	5.2
1	A	76	SER	5.0
1	F	89	PRO	4.9
3	E	54	GLN	4.8
1	A	55	ILE	4.6
3	J	57	LYS	4.5
1	F	53	PHE	4.4
3	E	56	HIS	4.3
1	A	45	GLN	4.3
1	A	109	LEU	4.3
1	A	110	LEU	4.2
3	E	58	SER	4.2
1	A	89	PRO	4.2
2	G	-9	GLY	4.2
1	A	57	PRO	4.2
6	O	28	GLU	4.1
1	F	20	ALA	4.0
3	J	58	SER	3.9
2	G	-4	PHE	3.9
1	F	61	TRP	3.9
1	A	111	ILE	3.8
1	F	83	LEU	3.8
1	F	84	LEU	3.8
3	E	55	GLY	3.7
1	F	117	LEU	3.7
1	F	56	ASP	3.6
1	F	135	VAL	3.6
1	F	110	LEU	3.6
1	A	82	LEU	3.6
1	A	80	LEU	3.6
1	F	9	LEU	3.5
3	E	57	LYS	3.5
1	F	19	ALA	3.5
1	F	2	ILE	3.5
1	A	41	VAL	3.4
1	F	123	ASN	3.4
1	A	108	LEU	3.4
2	G	-3	GLN	3.3
1	F	10	ARG	3.3
1	F	87	ASN	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	22	LEU	3.3
1	A	56	ASP	3.3
1	F	3	ARG	3.2
1	A	62	ASN	3.2
1	A	75	ALA	3.2
1	A	104	LEU	3.2
1	F	134	SER	3.2
1	A	79	THR	3.1
1	F	6	PRO	3.1
3	J	59	CYS	3.1
1	F	67	LEU	3.0
1	F	136	GLN	3.0
2	D	302	LEU	3.0
2	G	-5	LEU	3.0
1	F	128	THR	2.9
1	F	21	TYR	2.9
1	A	101	THR	2.9
1	F	82	LEU	2.9
1	F	60	ASP	2.9
2	G	-6	VAL	2.9
1	A	60	ASP	2.8
1	F	88	GLY	2.8
1	F	119	LYS	2.8
1	A	1	MET	2.7
1	A	107	ASP	2.7
1	A	21	TYR	2.7
1	A	15	GLU	2.7
1	A	81	LEU	2.7
4	K	3	DT	2.6
6	P	28	GLU	2.6
1	A	196	LYS	2.6
1	F	129	ALA	2.6
1	A	112	VAL	2.5
1	F	107	ASP	2.5
2	I	227	SER	2.5
3	E	60	GLY	2.5
1	F	59	THR	2.5
1	F	62	ASN	2.5
1	A	34	SER	2.5
1	A	68	CYS	2.5
1	F	58	ASN	2.5
2	D	304	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	127	PHE	2.5
2	G	-7	GLU	2.4
1	F	69	GLN	2.4
1	F	22	LEU	2.4
2	I	362	ARG	2.4
4	K	2	DT	2.4
2	G	88	VAL	2.4
1	A	74	PHE	2.4
1	F	7	GLU	2.4
2	I	75	VAL	2.4
1	F	132	ASN	2.3
1	F	8	GLN	2.2
1	A	20	ALA	2.2
1	F	4	LEU	2.2
1	A	48	GLU	2.2
1	F	120	ALA	2.2
1	F	109	LEU	2.2
1	A	78	GLN	2.2
1	A	113	ARG	2.2
2	B	204	GLN	2.2
2	C	248	GLN	2.2
1	F	133	ARG	2.1
1	A	77	ARG	2.1
1	F	13	LEU	2.1
1	F	111	ILE	2.1
2	G	222	ASP	2.0
3	J	48	LEU	2.0
1	A	106	ASP	2.0
1	F	97	LEU	2.0
1	F	113	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	MG	H	416	1/1	0.96	0.34	5.02	66,66,66,66	0
9	MG	B	412	1/1	0.96	0.26	2.27	86,86,86,86	0
8	BEF	C	403	4/4	0.96	0.28	1.93	85,86,86,87	0
9	MG	C	413	1/1	0.96	0.27	1.64	83,83,83,83	0
8	BEF	H	409	4/4	0.94	0.26	0.92	74,74,74,75	0
9	MG	D	414	1/1	0.92	0.28	0.67	83,83,83,83	0
9	MG	I	417	1/1	0.96	0.28	0.66	67,67,67,67	0
9	MG	G	415	1/1	0.89	0.28	0.49	92,92,92,92	0
7	ADP	H	408	27/27	0.98	0.25	0.14	70,73,78,78	0
7	ADP	B	400	27/27	0.95	0.25	-0.32	92,101,107,110	0
7	ADP	C	402	27/27	0.97	0.23	-0.33	87,94,101,102	0
10	ZN	H	423	1/1	0.98	0.13	-0.44	153,153,153,153	0
8	BEF	D	405	4/4	0.91	0.21	-0.54	81,82,82,83	0
7	ADP	G	406	27/27	0.95	0.24	-0.55	93,100,105,107	0
7	ADP	I	410	27/27	0.96	0.25	-0.63	67,74,77,79	0
8	BEF	B	401	4/4	0.97	0.21	-0.65	96,96,96,97	0
8	BEF	I	411	4/4	0.95	0.21	-0.72	81,81,82,83	0
7	ADP	D	404	27/27	0.95	0.21	-0.87	84,93,99,101	0
10	ZN	E	421	1/1	0.85	0.17	-1.04	267,267,267,267	0
10	ZN	I	424	1/1	0.97	0.11	-1.22	107,107,107,107	0
10	ZN	C	419	1/1	0.99	0.12	-1.25	146,146,146,146	0
8	BEF	G	407	4/4	0.95	0.20	-1.41	94,94,94,95	0
10	ZN	J	425	1/1	0.79	0.21	-1.68	253,253,253,253	0
10	ZN	B	418	1/1	0.98	0.06	-1.93	162,162,162,162	0
10	ZN	G	422	1/1	1.00	0.08	-2.10	178,178,178,178	0
10	ZN	D	420	1/1	0.98	0.06	-2.41	144,144,144,144	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.