



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:27 pm BST

PDB ID : 3RMA  
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing  
Thymine Glycol  
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.  
Deposited on : 2011-04-20  
Resolution : 2.84 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

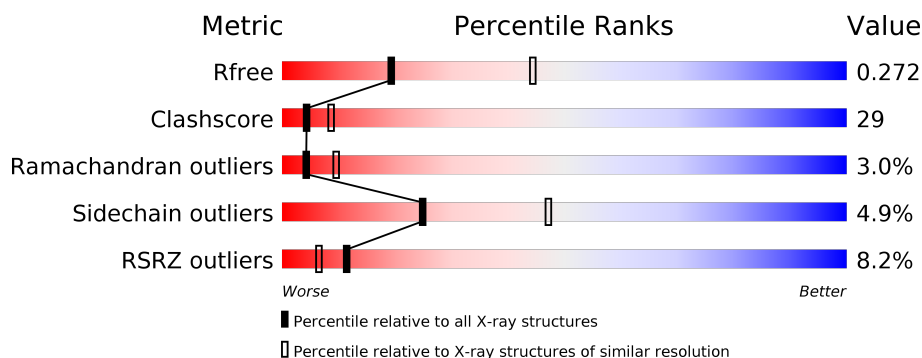
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	906	<div> <div>3%</div> <div>60%</div> <div>37%</div> <div>..</div> </div>
1	B	906	<div> <div>14%</div> <div>53%</div> <div>42%</div> <div>..</div> </div>
1	C	906	<div> <div>2%</div> <div>59%</div> <div>35%</div> <div>..</div> </div>
1	D	906	<div> <div>13%</div> <div>39%</div> <div>52%</div> <div>7%</div> <div>.</div> </div>
2	E	18	<div> <div>22%</div> <div>56%</div> <div>22%</div> </div>
2	G	18	<div> <div>17%</div> <div>6%</div> <div>67%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	18	<div><div></div><div>39%</div><div>50%</div><div>6%</div><div>6%</div></div>
2	K	18	<div><div>6%</div><div>17%</div><div>50%</div><div>33%</div></div>
3	F	14	<div><div></div><div>29%</div><div>71%</div></div>
3	H	14	<div><div>7%</div><div>21%</div><div>71%</div><div>7%</div></div>
3	J	14	<div><div></div><div>14%</div><div>86%</div></div>
3	L	14	<div><div></div><div>21%</div><div>71%</div><div>7%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31451 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	894	Total	C	N	O	S	4	0	0
			7273	4672	1207	1362	32			
1	B	897	Total	C	N	O	S	62	0	0
			7230	4645	1200	1353	32			
1	C	890	Total	C	N	O	S	8	0	0
			7227	4642	1198	1356	31			
1	D	890	Total	C	N	O	S	20	0	0
			7161	4599	1190	1341	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	904	HIS	-	EXPRESSION TAG	UNP Q38087
A	905	HIS	-	EXPRESSION TAG	UNP Q38087
A	906	HIS	-	EXPRESSION TAG	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	904	HIS	-	EXPRESSION TAG	UNP Q38087
B	905	HIS	-	EXPRESSION TAG	UNP Q38087
B	906	HIS	-	EXPRESSION TAG	UNP Q38087
C	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	904	HIS	-	EXPRESSION TAG	UNP Q38087
C	905	HIS	-	EXPRESSION TAG	UNP Q38087
C	906	HIS	-	EXPRESSION TAG	UNP Q38087
D	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	904	HIS	-	EXPRESSION TAG	UNP Q38087
D	905	HIS	-	EXPRESSION TAG	UNP Q38087
D	906	HIS	-	EXPRESSION TAG	UNP Q38087

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			287	136	59	79	13			
2	G	13	Total	C	N	O	P	0	0	0
			265	126	54	73	12			
2	I	17	Total	C	N	O	P	0	0	0
			352	166	71	99	16			
2	K	12	Total	C	N	O	P	0	0	0
			244	116	49	68	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			282	136	50	83	13			
3	H	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			
3	J	14	Total	C	N	O	P	0	0	0
			282	136	50	83	13			
3	L	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	61	Total	O	0	0
			61	61		
4	C	99	Total	O	0	0
			99	99		
4	D	16	Total	O	0	0
			16	16		
4	E	5	Total	O	0	0
			5	5		
4	F	2	Total	O	0	0
			2	2		
4	G	4	Total	O	0	0
			4	4		
4	H	4	Total	O	0	0
			4	4		

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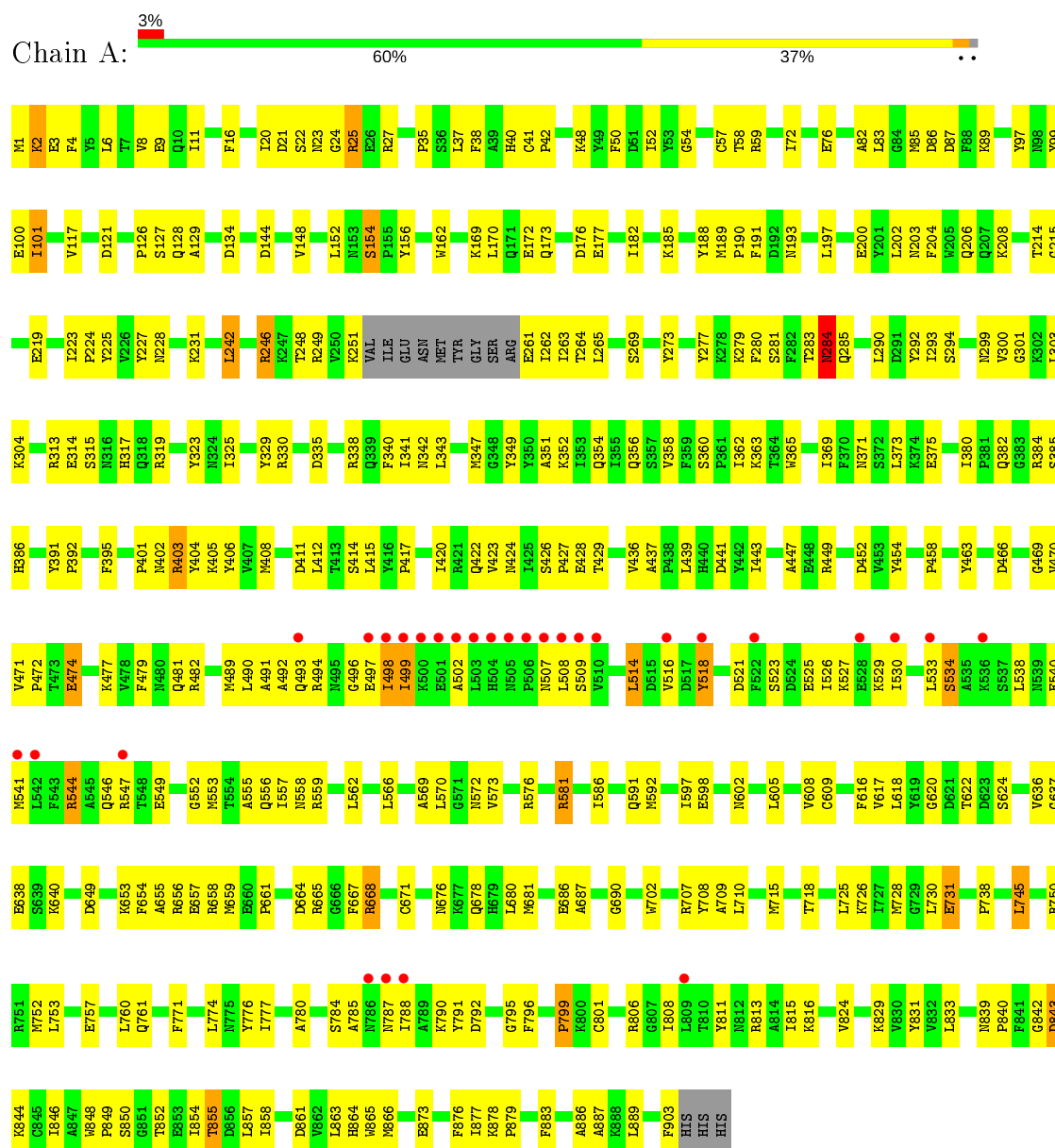
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	7	Total	O	0	0
			7	7		
4	J	6	Total	O	0	0
			6	6		
4	K	6	Total	O	0	0
			6	6		

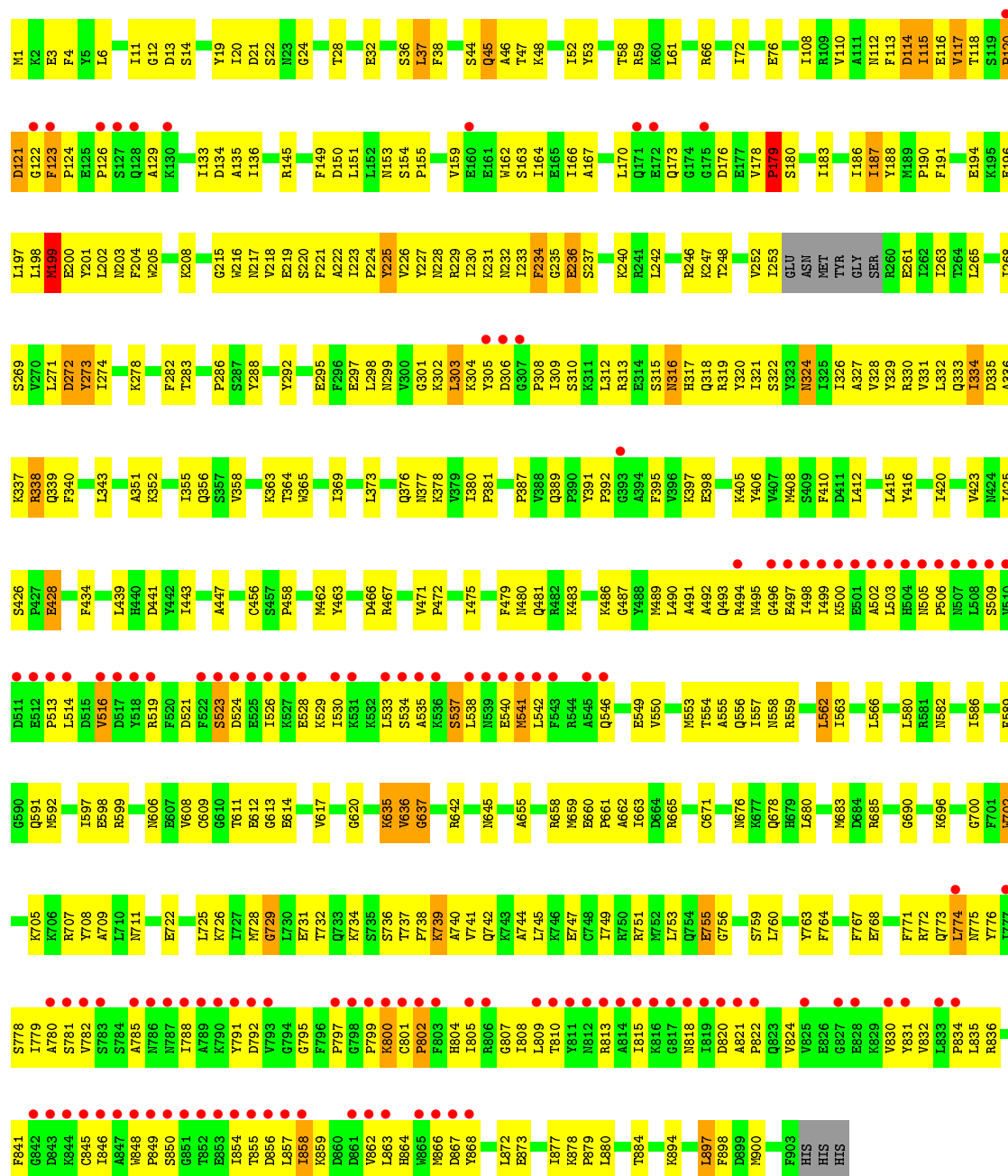
### 3 Residue-property plots

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

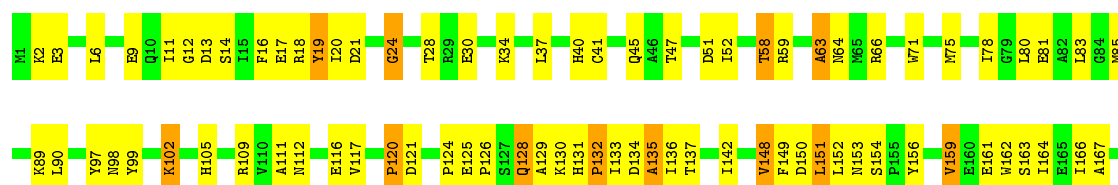
- Molecule 1: DNA polymerase



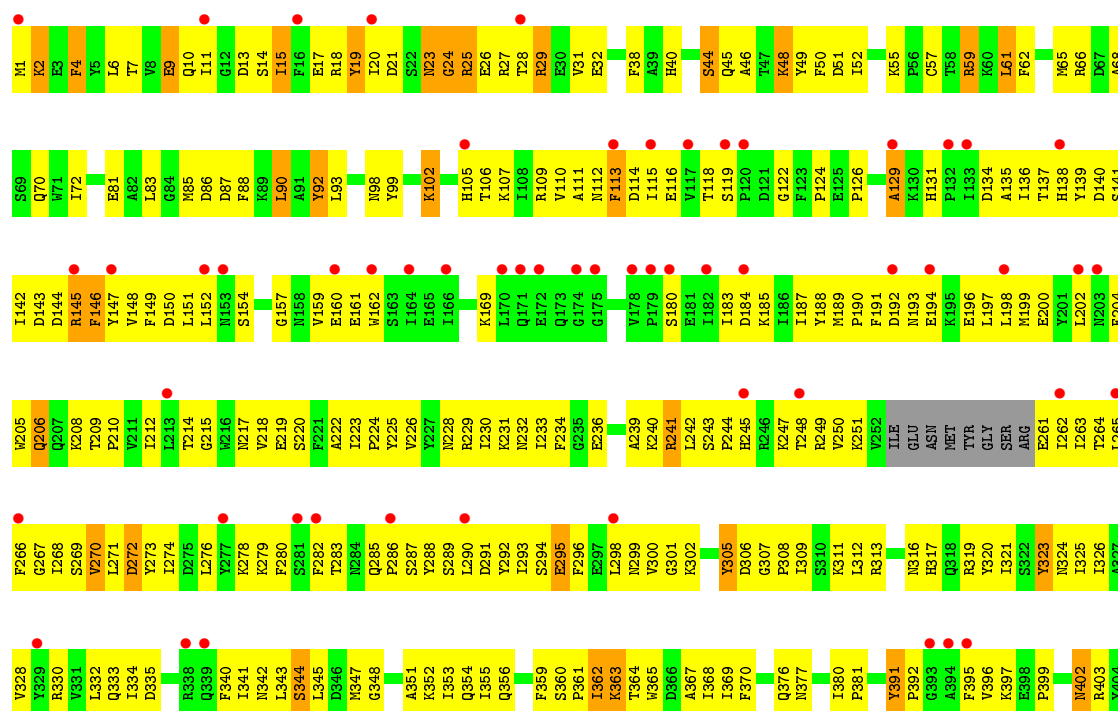
- Molecule 1: DNA polymerase

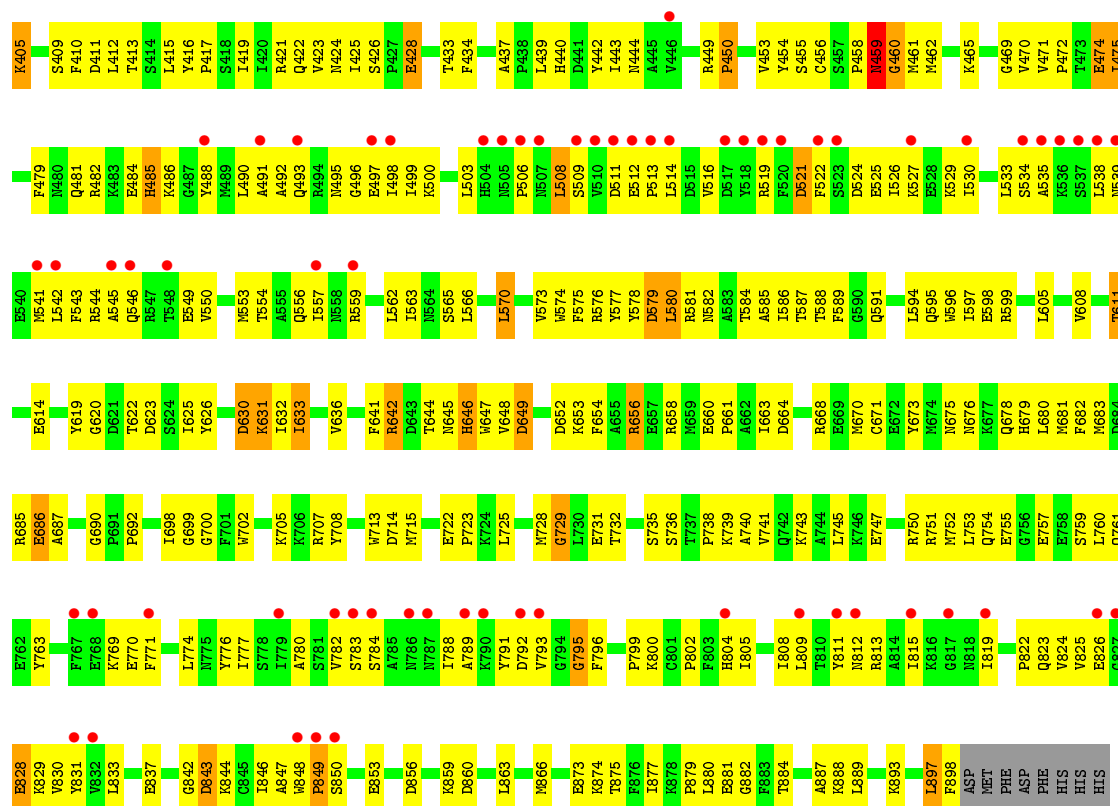


• Molecule 1: DNA polymerase



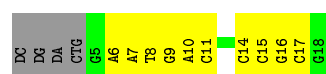






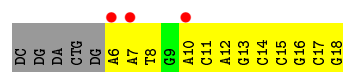
• Molecule 2: DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain E: 22% 56% 22%



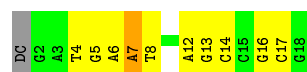
• Molecule 2: DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain G: 6% 17% 67% 28%

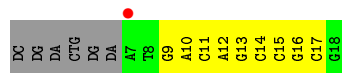
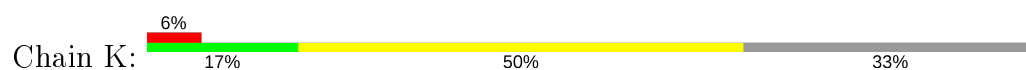


• Molecule 2: DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain I: 39% 50% 6% 6%



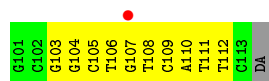
• Molecule 2: DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')



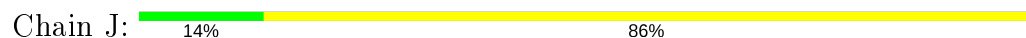
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*A)-3')



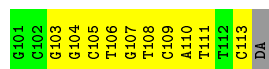
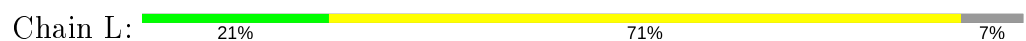
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*A)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.70 Å 123.00 Å 163.94 Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.84 49.09 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.84) 98.2 (49.09-2.84)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.215 , 0.275 0.214 , 0.272	Depositor DCC
$R_{free}$ test set	23396 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CTG

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	0.45	0/7452	0.65	0/10078
1	B	0.38	0/7405	0.60	0/10021
1	C	0.42	0/7404	0.63	0/10015
1	D	0.32	0/7337	0.55	0/9939
2	E	0.34	0/323	0.68	0/497
2	G	0.33	0/298	0.70	0/458
2	I	0.55	0/371	0.74	0/569
2	K	0.31	0/274	0.66	0/421
3	F	0.29	0/315	0.69	0/484
3	H	0.25	0/292	0.65	0/449
3	J	0.48	0/315	0.73	0/484
3	L	0.28	0/292	0.65	0/449
All	All	0.39	0/32078	0.62	0/43864

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	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	7	DA	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7273	0	7125	292	0
1	B	7230	0	7057	418	0
1	C	7227	0	7083	327	0
1	D	7161	0	6961	604	0
2	E	287	0	157	17	0
2	G	265	0	146	22	0
2	I	352	0	193	11	0
2	K	244	0	135	16	0
3	F	282	0	158	19	0
3	H	262	0	149	22	0
3	J	282	0	158	20	0
3	L	262	0	149	17	0
4	A	114	0	0	6	0
4	B	61	0	0	3	0
4	C	99	0	0	3	0
4	D	16	0	0	3	0
4	E	5	0	0	2	0
4	F	2	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	1	0
4	I	7	0	0	1	0
4	J	6	0	0	0	0
4	K	6	0	0	1	0
All	All	31451	0	29471	1758	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1758) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HD2	1:A:2:LYS:H	1.13	1.10
1:D:422:GLN:HE22	1:D:681:MET:HG2	1.15	1.09
1:D:481:GLN:HB3	1:D:559:ARG:HE	1.14	1.07
1:D:85:MET:HE2	1:D:87:ASP:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:16:DG:H2''	2:K:17:DC:H5''	1.37	1.05
1:B:818:ASN:HD21	1:B:857:LEU:HD11	1.17	1.05
1:B:731:GLU:HA	1:B:734:LYS:HG2	1.39	1.04
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.32	1.04
1:B:707:ARG:HE	2:G:8:DT:H4'	1.18	1.04
1:D:543:PHE:HA	1:D:546:GLN:HE21	1.20	1.02
1:D:90:LEU:HD11	1:D:353:ILE:HG22	1.43	1.01
1:A:85:MET:HE2	1:A:87:ASP:H	1.23	1.00
1:D:516:VAL:HG11	1:D:526:ILE:HG21	1.42	1.00
1:B:136:ILE:HG23	1:B:149:PHE:HB2	1.42	0.98
1:D:295:GLU:HG2	1:D:301:GLY:HA2	1.43	0.97
1:A:857:LEU:HD12	1:A:858:ILE:HG23	1.46	0.96
1:A:395:PHE:HB2	1:A:591:GLN:HG3	1.47	0.96
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.43	0.96
1:C:482:ARG:HE	1:C:556:GLN:HE21	1.13	0.96
1:A:482:ARG:NE	1:A:556:GLN:HE21	1.64	0.96
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.47	0.96
1:C:130:LYS:HG3	1:C:131:HIS:H	1.28	0.95
1:D:859:LYS:HG3	1:D:860:ASP:H	1.30	0.95
1:B:481:GLN:HE21	1:B:559:ARG:HE	1.08	0.95
1:D:112:ASN:HB3	1:D:214:THR:HG23	1.45	0.95
1:D:500:LYS:HA	1:D:503:LEU:HB2	1.49	0.95
1:B:395:PHE:HB2	1:B:591:GLN:HG2	1.49	0.94
1:C:395:PHE:HB2	1:C:591:GLN:HG3	1.49	0.94
1:B:606:ASN:HD21	1:B:614:GLU:H	1.15	0.94
1:A:482:ARG:HE	1:A:556:GLN:HE21	0.98	0.94
1:B:815:ILE:HD11	1:B:855:THR:HG21	1.50	0.94
1:C:354:GLN:HB3	1:C:356:GLN:HE22	1.33	0.94
1:B:387:PRO:HG2	1:B:389:GLN:HE21	1.30	0.93
1:C:461:MET:HE3	1:C:581:ARG:HD2	1.46	0.93
3:L:108:DT:H2''	3:L:109:DC:H5''	1.51	0.93
2:K:15:DC:H2''	2:K:16:DG:C8	2.04	0.92
1:B:514:LEU:H	1:B:541:MET:HE3	1.34	0.92
1:D:573:VAL:HG23	1:D:574:TRP:HD1	1.35	0.92
2:G:10:DA:H2''	2:G:11:DC:H5'	1.51	0.92
2:K:10:DA:H2''	2:K:11:DC:H5''	1.53	0.91
1:A:514:LEU:HD12	1:A:530:ILE:HG12	1.53	0.91
1:D:449:ARG:HH21	1:D:675:ASN:HB2	1.36	0.91
1:C:486:LYS:HB2	1:C:556:GLN:HG3	1.53	0.91
2:E:10:DA:H2''	2:E:11:DC:H5'	1.54	0.90
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:ARG:HB2	1:D:559:ARG:HB3	1.53	0.88
1:D:9:GLU:HB3	1:D:11:ILE:HD11	1.56	0.87
3:F:104:DG:H1'	3:F:105:DC:H5''	1.55	0.87
1:D:261:GLU:HG3	1:D:262:ILE:HG13	1.54	0.87
1:D:752:MET:HG2	1:D:760:LEU:HD12	1.58	0.86
1:D:481:GLN:CB	1:D:559:ARG:HE	1.89	0.86
1:D:543:PHE:HA	1:D:546:GLN:NE2	1.89	0.86
1:B:606:ASN:HD22	1:B:612:GLU:HA	1.39	0.86
1:D:118:THR:HB	1:D:313:ARG:HE	1.40	0.85
1:D:288:TYR:HA	1:D:293:ILE:HD11	1.57	0.85
1:B:170:LEU:HB2	1:B:173:GLN:HE21	1.42	0.85
1:D:206:GLN:HE22	1:D:241:ARG:HB3	1.42	0.85
1:B:894:LYS:HA	4:B:918:HOH:O	1.77	0.84
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.42	0.84
1:B:163:SER:H	1:B:318:GLN:HE22	1.22	0.84
1:D:812:ASN:HA	1:D:815:ILE:HG12	1.60	0.84
1:A:3:GLU:HG2	1:A:21:ASP:HA	1.60	0.84
1:C:645:ASN:HD21	1:C:719:ARG:HD2	1.42	0.84
1:A:449:ARG:HH12	1:A:452:ASP:HB3	1.42	0.83
1:B:897:LEU:H	1:B:897:LEU:HD23	1.41	0.83
1:B:707:ARG:NE	2:G:8:DT:H4'	1.93	0.83
1:D:81:GLU:OE1	1:D:83:LEU:HD21	1.77	0.83
1:B:115:ILE:HG12	1:B:116:GLU:H	1.44	0.82
1:D:656:ARG:HA	1:D:660:GLU:OE2	1.79	0.82
1:B:145:ARG:HD2	1:B:187:ILE:HD11	1.60	0.82
3:J:113:DC:H2''	3:J:114:DA:H5''	1.61	0.82
3:H:104:DG:H2''	3:H:105:DC:H5''	1.62	0.82
1:C:495:ASN:HD21	1:C:521:ASP:HA	1.44	0.81
1:B:217:ASN:HB2	1:B:274:ILE:HD12	1.62	0.81
1:D:222:ALA:O	1:D:226:VAL:HG23	1.80	0.81
1:B:502:ALA:HB3	1:B:530:ILE:HG12	1.61	0.81
1:D:503:LEU:O	1:D:506:PRO:HD3	1.81	0.81
1:A:499:ILE:HD13	1:A:541:MET:HG3	1.61	0.81
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.62	0.81
1:C:424:ASN:HD21	1:C:469:GLY:H	1.24	0.81
1:A:206:GLN:HE22	1:A:246:ARG:NH2	1.79	0.80
1:B:493:GLN:HB3	1:B:549:GLU:OE2	1.81	0.80
1:D:271:LEU:HB3	1:D:276:LEU:HD11	1.60	0.80
1:D:402:ASN:ND2	1:D:403:ARG:H	1.80	0.80
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.46	0.80
1:D:302:LYS:HE3	1:D:323:TYR:HE2	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:PHE:HB2	1:D:591:GLN:HG3	1.63	0.80
1:C:544:ARG:HG2	1:C:547:ARG:HH21	1.47	0.79
1:D:831:TYR:HD2	1:D:848:TRP:HE1	1.27	0.79
1:D:361:PRO:HB3	1:D:565:SER:HB2	1.65	0.79
1:C:249:ARG:HD3	1:C:251:LYS:NZ	1.96	0.79
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.63	0.79
1:C:382:GLN:HG2	1:C:383:GLY:N	1.98	0.79
2:K:16:DG:C2'	2:K:17:DC:H5''	2.13	0.79
1:C:216:TRP:O	1:C:217:ASN:HB2	1.82	0.79
1:D:298:LEU:HB2	1:D:300:VAL:HG12	1.63	0.79
1:D:542:LEU:O	1:D:546:GLN:HG3	1.83	0.79
2:G:15:DC:H2'	2:G:16:DG:C8	2.17	0.79
1:B:115:ILE:HD11	1:B:133:ILE:HG12	1.65	0.79
1:D:434:PHE:CE1	1:D:460:GLY:HA2	2.18	0.79
3:L:108:DT:C2'	3:L:109:DC:H5''	2.13	0.78
1:C:382:GLN:HG2	1:C:383:GLY:H	1.46	0.78
1:D:236:GLU:HA	1:D:239:ALA:HB3	1.66	0.78
1:D:6:LEU:HG	1:D:19:TYR:HA	1.63	0.78
1:D:308:PRO:HG2	1:D:311:LYS:HB2	1.64	0.77
1:B:123:PHE:CE1	1:B:309:ILE:HD11	2.19	0.77
1:A:428:GLU:OE2	1:A:470:VAL:HG23	1.85	0.77
1:C:219:GLU:HG3	1:C:270:VAL:HG11	1.66	0.77
1:D:516:VAL:HG21	1:D:522:PHE:CZ	2.20	0.77
1:A:249:ARG:HH11	1:A:251:LYS:HE2	1.49	0.77
1:B:115:ILE:HD11	1:B:133:ILE:CG1	2.15	0.77
1:D:825:VAL:HB	1:D:828:GLU:HB2	1.66	0.76
1:B:854:ILE:HD13	1:B:862:VAL:HG11	1.67	0.76
1:D:830:VAL:HG23	1:D:848:TRP:O	1.85	0.76
1:B:785:ALA:HB1	1:B:788:ILE:HD11	1.67	0.76
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.21	0.76
3:F:108:DT:H2''	3:F:109:DC:H5''	1.66	0.76
1:A:283:THR:O	1:A:285:GLN:HG2	1.85	0.76
1:D:205:TRP:NE1	1:D:242:LEU:HA	2.01	0.76
3:H:104:DG:H2''	3:H:105:DC:C5'	2.15	0.76
1:C:130:LYS:HG3	1:C:131:HIS:N	2.01	0.76
1:A:314:GLU:HG3	1:A:315:SER:N	2.00	0.76
1:A:482:ARG:HE	1:A:556:GLN:NE2	1.81	0.76
1:B:776:TYR:HB3	1:B:863:LEU:HD13	1.68	0.76
1:D:644:THR:O	1:D:648:VAL:HG23	1.86	0.76
1:D:859:LYS:HG3	1:D:860:ASP:N	2.01	0.76
2:G:10:DA:H2''	2:G:11:DC:C5'	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:O	1:A:76:GLU:HG3	1.86	0.75
1:C:481:GLN:HE21	1:C:559:ARG:HE	1.32	0.75
1:D:530:ILE:HG13	1:D:533:LEU:HD22	1.68	0.75
1:B:533:LEU:HB2	1:B:538:LEU:HD13	1.67	0.75
1:A:602:ASN:HD21	1:A:617:VAL:H	1.35	0.75
1:B:163:SER:HB3	1:B:166:ILE:HB	1.68	0.75
1:B:736:SER:HA	1:B:782:VAL:HB	1.68	0.75
1:D:295:GLU:CG	1:D:301:GLY:HA2	2.16	0.75
1:A:281:SER:HB2	1:A:338:ARG:HH21	1.52	0.74
1:A:290:LEU:O	1:A:294:SER:HB2	1.86	0.74
1:B:322:SER:O	1:B:326:ILE:HG12	1.87	0.74
1:C:303:LEU:HD23	1:C:323:TYR:HB2	1.69	0.74
1:D:229:ARG:HG3	1:D:233:ILE:HD11	1.69	0.74
1:A:502:ALA:O	1:A:538:LEU:HD13	1.87	0.74
1:B:115:ILE:HG12	1:B:116:GLU:N	2.01	0.74
1:C:326:ILE:HD12	1:C:327:ALA:N	2.03	0.74
2:E:6:DA:H1'	2:E:7:DA:H5''	1.70	0.74
1:A:526:ILE:HG22	1:A:530:ILE:HD11	1.69	0.74
1:B:897:LEU:HD12	1:D:636:VAL:HG11	1.68	0.74
1:D:145:ARG:HG3	1:D:185:LYS:O	1.88	0.74
1:D:15:ILE:HD12	1:D:92:TYR:CE2	2.21	0.74
2:K:10:DA:C2'	2:K:11:DC:H5''	2.17	0.74
1:D:411:ASP:HB2	1:D:686:GLU:OE1	1.88	0.74
1:B:481:GLN:HE21	1:B:559:ARG:NE	1.82	0.73
1:D:25:ARG:HG3	1:D:25:ARG:HH11	1.53	0.73
1:B:658:ARG:HD2	1:D:897:LEU:HD22	1.70	0.73
1:C:78:ILE:HG13	1:C:80:LEU:HD23	1.70	0.73
1:D:343:LEU:HD23	1:D:554:THR:HG23	1.67	0.73
1:D:805:ILE:HA	1:D:808:ILE:HD12	1.71	0.73
1:B:170:LEU:HB2	1:B:173:GLN:NE2	2.04	0.73
1:D:85:MET:HE2	1:D:87:ASP:N	2.01	0.73
1:D:109:ARG:HD2	1:D:209:THR:O	1.88	0.73
1:D:751:ARG:HD3	1:D:759:SER:OG	1.87	0.73
2:K:10:DA:H2''	2:K:11:DC:C5'	2.19	0.73
3:L:108:DT:H2''	3:L:109:DC:C5'	2.19	0.73
1:B:116:GLU:HG3	1:B:135:ALA:HB3	1.69	0.72
1:D:525:GLU:O	1:D:529:LYS:HE2	1.89	0.72
1:A:362:ILE:HD12	1:A:569:ALA:HA	1.71	0.72
1:A:428:GLU:N	1:A:428:GLU:OE1	2.22	0.72
1:A:449:ARG:NH1	1:A:452:ASP:HB3	2.04	0.72
1:B:738:PRO:HG2	1:B:741:VAL:HB	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:PHE:O	1:D:658:ARG:HB2	1.88	0.72
3:H:104:DG:C2'	3:H:105:DC:H5''	2.19	0.72
1:B:486:LYS:HG3	1:B:556:GLN:OE1	1.88	0.72
1:D:271:LEU:HD22	1:D:276:LEU:HD21	1.69	0.72
1:B:327:ALA:O	1:B:331:VAL:HG23	1.90	0.72
1:D:151:LEU:HD23	1:D:152:LEU:N	2.05	0.72
1:B:731:GLU:HA	1:B:734:LYS:CG	2.18	0.72
1:D:66:ARG:O	1:D:70:GLN:HG2	1.89	0.72
1:A:842:GLY:O	1:A:843:ASP:HB2	1.90	0.72
1:D:508:LEU:HD22	1:D:508:LEU:H	1.55	0.72
1:D:461:MET:CE	1:D:581:ARG:HH21	2.02	0.72
1:A:530:ILE:O	1:A:533:LEU:HD13	1.90	0.71
1:C:163:SER:H	1:C:318:GLN:HE22	1.36	0.71
1:C:354:GLN:HB3	1:C:356:GLN:NE2	2.05	0.71
3:J:104:DG:H1'	3:J:105:DC:H5''	1.71	0.71
1:D:481:GLN:HB3	1:D:559:ARG:NE	1.98	0.71
1:D:313:ARG:HD3	1:D:320:TYR:CE2	2.26	0.71
1:D:302:LYS:HE3	1:D:323:TYR:CE2	2.26	0.71
1:A:362:ILE:CD1	1:A:569:ALA:HA	2.21	0.71
3:J:108:DT:H2''	3:J:109:DC:H5'	1.71	0.71
1:A:449:ARG:HH12	1:A:452:ASP:CB	2.04	0.71
1:B:330:ARG:O	1:B:334:ILE:HG22	1.90	0.71
1:B:795:GLY:O	1:B:813:ARG:HD3	1.91	0.71
1:D:316:ASN:HD22	1:D:319:ARG:HB3	1.56	0.71
1:D:330:ARG:O	1:D:334:ILE:HG13	1.91	0.71
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.72	0.70
1:D:550:VAL:HA	1:D:553:MET:HB3	1.73	0.70
2:E:6:DA:H2''	2:E:7:DA:H5'	1.72	0.70
1:C:815:ILE:HD12	1:C:821:ALA:CB	2.21	0.70
1:D:229:ARG:O	1:D:233:ILE:HG13	1.90	0.70
1:D:360:SER:HB2	1:D:363:LYS:HB2	1.73	0.70
1:A:206:GLN:HE22	1:A:246:ARG:HH22	1.39	0.70
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.26	0.70
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.56	0.70
1:B:1:MET:HE1	1:B:24:GLY:HA2	1.73	0.70
2:G:16:DG:H2''	2:G:17:DC:C5'	2.22	0.70
1:B:818:ASN:ND2	1:B:857:LEU:HD11	2.01	0.70
1:D:160:GLU:HG3	1:D:161:GLU:H	1.57	0.70
1:D:422:GLN:NE2	1:D:681:MET:HG2	2.00	0.70
1:A:422:GLN:NE2	1:A:680:LEU:H	1.89	0.70
1:B:334:ILE:HG13	1:B:338:ARG:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLN:H	1:C:356:GLN:HE21	1.40	0.70
1:D:359:PHE:O	1:D:361:PRO:HD3	1.92	0.70
1:B:513:PRO:HG2	1:B:540:GLU:HG3	1.74	0.69
1:D:137:THR:H	1:D:324:ASN:HD21	1.38	0.69
1:B:744:ALA:HB2	1:B:767:PHE:CE2	2.28	0.69
1:D:479:PHE:HA	1:D:563:ILE:HD11	1.74	0.69
2:E:10:DA:H2''	2:E:11:DC:C5'	2.22	0.69
1:D:191:PHE:CD2	1:D:197:LEU:HA	2.27	0.69
1:A:224:PRO:HA	1:A:263:ILE:HD13	1.75	0.69
1:B:554:THR:HA	1:B:557:ILE:HG22	1.75	0.69
1:C:645:ASN:ND2	1:C:719:ARG:HD2	2.08	0.69
1:D:305:TYR:CG	1:D:312:LEU:HD22	2.27	0.69
1:B:136:ILE:CG2	1:B:149:PHE:HB2	2.19	0.69
1:D:198:LEU:HD23	1:D:230:ILE:HG12	1.75	0.69
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.08	0.69
1:D:191:PHE:CZ	1:D:200:GLU:HB3	2.27	0.69
1:D:642:ARG:HD2	1:D:646:HIS:CE1	2.28	0.69
1:A:558:ASN:O	1:A:562:LEU:HD22	1.93	0.68
1:B:188:TYR:CZ	1:B:190:PRO:HB3	2.28	0.68
1:B:72:ILE:O	1:B:76:GLU:HG3	1.92	0.68
1:B:846:ILE:HG21	1:B:862:VAL:HG23	1.75	0.68
1:D:205:TRP:HE1	1:D:242:LEU:HA	1.59	0.68
1:D:402:ASN:HD22	1:D:403:ARG:H	1.42	0.68
1:B:272:ASP:OD1	1:B:274:ILE:HG22	1.94	0.68
1:B:481:GLN:NE2	1:B:559:ARG:HE	1.88	0.68
1:D:402:ASN:ND2	1:D:403:ARG:HG2	2.08	0.68
1:A:281:SER:HB2	1:A:338:ARG:NH2	2.08	0.68
1:D:738:PRO:HB3	1:D:780:ALA:O	1.92	0.68
1:B:554:THR:HA	1:B:557:ILE:CG2	2.24	0.68
1:A:261:GLU:O	1:A:262:ILE:HD12	1.95	0.67
1:A:281:SER:O	1:A:283:THR:HG23	1.94	0.67
1:B:129:ALA:HB1	1:B:225:TYR:CE2	2.29	0.67
1:D:31:VAL:HG12	1:D:32:GLU:N	2.08	0.67
1:D:793:VAL:HG22	1:D:796:PHE:O	1.94	0.67
1:A:402:ASN:HA	1:A:886:ALA:O	1.93	0.67
3:F:108:DT:H2''	3:F:109:DC:C5'	2.24	0.67
1:C:83:LEU:N	1:C:83:LEU:HD12	2.09	0.67
1:D:403:ARG:HD2	1:D:887:ALA:O	1.93	0.67
1:B:116:GLU:CG	1:B:135:ALA:HB3	2.25	0.67
1:D:316:ASN:ND2	1:D:319:ARG:HB3	2.10	0.67
1:C:818:ASN:ND2	1:C:857:LEU:HD11	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:CZ	1:D:142:ILE:HD11	2.25	0.67
1:D:434:PHE:HE1	1:D:461:MET:H	1.41	0.67
1:C:152:LEU:HD11	1:C:161:GLU:HG2	1.76	0.66
1:D:340:PHE:HD1	1:D:343:LEU:HD12	1.60	0.66
1:A:855:THR:HG23	1:A:858:ILE:HG12	1.77	0.66
1:C:645:ASN:ND2	1:C:719:ARG:HH11	1.93	0.66
1:D:7:THR:HG22	1:D:18:ARG:HB2	1.78	0.66
1:D:219:GLU:OE2	1:D:262:ILE:HG23	1.94	0.66
1:D:453:VAL:HG23	1:D:454:TYR:CD2	2.30	0.66
2:G:15:DC:H42	3:H:103:DG:H1	1.43	0.66
1:A:2:LYS:HD2	1:A:2:LYS:N	1.97	0.66
1:A:82:ALA:O	1:A:382:GLN:HB2	1.95	0.66
1:A:474:GLU:OE2	1:A:477:LYS:HE2	1.95	0.66
3:F:103:DG:H2''	3:F:104:DG:H5'	1.78	0.66
1:B:848:TRP:CE3	1:B:854:ILE:HD12	2.31	0.66
1:C:166:ILE:HG22	1:C:175:GLY:HA2	1.76	0.66
1:D:124:PRO:HB3	1:D:131:HIS:HD2	1.61	0.66
1:D:212:ILE:HG22	1:D:212:ILE:O	1.96	0.66
1:D:365:TRP:CE2	1:D:566:LEU:HD23	2.31	0.66
1:D:611:THR:HB	1:D:614:GLU:OE1	1.96	0.66
1:B:14:SER:HB3	1:B:32:GLU:OE2	1.95	0.66
1:D:399:PRO:HB3	1:D:619:TYR:CD2	2.31	0.66
1:B:229:ARG:NE	1:B:233:ILE:HD11	2.10	0.65
1:B:316:ASN:ND2	1:B:319:ARG:H	1.93	0.65
1:D:273:TYR:HA	1:D:276:LEU:HD12	1.76	0.65
1:D:831:TYR:HD2	1:D:848:TRP:NE1	1.94	0.65
1:D:458:PRO:HB2	1:D:588:THR:HG22	1.77	0.65
1:C:512:GLU:HB3	1:C:513:PRO:HD2	1.78	0.65
1:C:642:ARG:HD2	1:C:646:HIS:NE2	2.11	0.65
2:K:16:DG:H2''	2:K:17:DC:C5'	2.21	0.65
1:A:172:GLU:CD	1:A:172:GLU:H	1.99	0.65
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.26	0.65
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.79	0.65
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.77	0.65
1:B:331:VAL:O	1:B:334:ILE:HG23	1.97	0.65
1:D:305:TYR:OH	1:D:309:ILE:HB	1.95	0.65
1:D:31:VAL:HG12	1:D:32:GLU:H	1.59	0.65
2:G:13:DG:H1	3:H:105:DC:H42	1.43	0.65
2:G:15:DC:H4'	2:G:15:DC:OP1	1.97	0.65
1:A:653:LYS:HD3	1:A:656:ARG:HH22	1.61	0.65
1:C:534:SER:O	1:C:538:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:HD21	1:B:318:GLN:HB3	1.62	0.65
1:B:52:ILE:HD12	1:B:428:GLU:HG3	1.79	0.65
1:C:660:GLU:CB	1:C:661:PRO:HD3	2.27	0.65
1:A:280:PHE:CD1	1:A:343:LEU:HD23	2.31	0.65
1:B:495:ASN:OD1	1:B:521:ASP:HA	1.97	0.65
1:D:137:THR:H	1:D:324:ASN:ND2	1.95	0.65
1:D:197:LEU:O	1:D:197:LEU:HD23	1.96	0.65
1:D:530:ILE:HA	1:D:533:LEU:HD13	1.77	0.65
3:L:110:DA:H1'	3:L:111:DT:H5''	1.76	0.65
1:C:486:LYS:HD3	1:C:556:GLN:NE2	2.12	0.65
1:C:818:ASN:HD22	1:C:821:ALA:H	1.45	0.65
3:J:104:DG:H2''	3:J:105:DC:C5'	2.27	0.65
1:B:123:PHE:CG	1:B:124:PRO:HD2	2.32	0.64
1:D:348:GLY:HA3	1:D:355:ILE:HD13	1.79	0.64
2:G:16:DG:H2''	2:G:17:DC:H5''	1.79	0.64
1:D:283:THR:CG2	1:D:285:GLN:HE22	2.09	0.64
1:D:353:ILE:HG13	1:D:354:GLN:O	1.96	0.64
1:D:802:PRO:HG2	1:D:805:ILE:CG1	2.27	0.64
2:E:14:DC:H2''	2:E:15:DC:O5'	1.97	0.64
1:B:808:ILE:HD11	1:B:830:VAL:HG21	1.80	0.64
1:D:248:THR:HG23	1:D:264:THR:O	1.96	0.64
1:D:740:ALA:O	1:D:743:LYS:HG2	1.97	0.64
1:D:825:VAL:HG12	1:D:826:GLU:N	2.12	0.64
1:D:131:HIS:HB2	1:D:225:TYR:OH	1.97	0.64
1:B:412:LEU:HD13	1:B:415:LEU:HD13	1.80	0.64
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.79	0.64
1:D:594:LEU:O	1:D:598:GLU:HG3	1.98	0.64
1:A:489:MET:SD	1:A:553:MET:HG2	2.37	0.64
1:B:229:ARG:CZ	1:B:233:ILE:HD11	2.28	0.64
1:D:271:LEU:HD13	1:D:276:LEU:HD21	1.79	0.64
1:A:314:GLU:CG	1:A:315:SER:N	2.61	0.64
1:B:164:ILE:HG22	1:B:183:ILE:HD11	1.79	0.64
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.80	0.64
1:D:148:VAL:HG21	1:D:325:ILE:HD11	1.80	0.64
1:D:625:ILE:HG12	1:D:683:MET:HE2	1.80	0.64
1:A:269:SER:OG	1:A:356:GLN:NE2	2.31	0.64
1:B:167:ALA:HB1	1:B:178:VAL:HG23	1.80	0.64
1:C:411:ASP:OD1	1:C:624:SER:HB3	1.98	0.64
1:D:191:PHE:HZ	1:D:200:GLU:HB3	1.61	0.64
1:D:812:ASN:HA	1:D:815:ILE:CG1	2.27	0.64
1:B:215:GLY:O	1:B:273:TYR:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:CB	1:B:591:GLN:HG2	2.26	0.64
1:C:482:ARG:NE	1:C:556:GLN:HE21	1.91	0.64
3:F:108:DT:C2'	3:F:109:DC:H5''	2.28	0.64
1:C:249:ARG:HD3	1:C:251:LYS:HZ3	1.61	0.63
1:D:250:VAL:HA	1:D:263:ILE:HD12	1.79	0.63
1:D:52:ILE:HD12	1:D:428:GLU:HG3	1.81	0.63
1:D:784:SER:HA	1:D:829:LYS:HA	1.80	0.63
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.34	0.63
1:B:490:LEU:HA	1:B:493:GLN:HG2	1.81	0.63
1:B:822:PRO:CG	1:B:855:THR:HB	2.28	0.63
1:C:3:GLU:HG2	1:C:21:ASP:HA	1.79	0.63
1:A:23:ASN:HD22	1:A:25:ARG:HH12	1.45	0.63
1:D:124:PRO:HB3	1:D:131:HIS:CD2	2.34	0.63
1:D:874:LYS:HG3	1:D:875:THR:HG23	1.81	0.63
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.80	0.63
1:B:499:ILE:HD12	1:B:530:ILE:HG13	1.81	0.63
1:C:815:ILE:HD12	1:C:821:ALA:HB1	1.80	0.63
1:A:362:ILE:HD11	1:A:572:ASN:HB3	1.81	0.62
1:A:343:LEU:HG	1:A:558:ASN:HD21	1.64	0.62
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.81	0.62
1:D:109:ARG:NH1	1:D:208:LYS:HB3	2.14	0.62
1:D:319:ARG:HG2	1:D:319:ARG:HH11	1.64	0.62
1:D:471:VAL:HG11	1:D:570:LEU:HD11	1.80	0.62
1:A:514:LEU:HD13	1:A:526:ILE:HG23	1.81	0.62
1:C:461:MET:HE3	1:C:581:ARG:CD	2.25	0.62
2:G:14:DC:H2''	2:G:15:DC:O5'	1.99	0.62
2:I:6:DA:H2''	2:I:7:DA:H5'	1.81	0.62
1:B:516:VAL:HG11	1:B:526:ILE:CD1	2.29	0.62
1:C:30:GLU:O	1:C:30:GLU:HG2	2.00	0.62
1:D:17:GLU:HG2	1:D:18:ARG:N	2.12	0.62
1:D:48:LYS:HD2	1:D:49:TYR:CE2	2.35	0.62
2:E:6:DA:H2''	2:E:7:DA:C5'	2.29	0.62
1:A:636:VAL:O	1:A:640:LYS:HD2	1.99	0.62
1:A:757:GLU:O	1:A:761:GLN:HG3	1.98	0.62
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.80	0.62
1:D:332:LEU:O	1:D:335:ASP:HB3	1.99	0.62
1:C:544:ARG:HG2	1:C:547:ARG:NH2	2.15	0.62
1:D:645:ASN:O	1:D:649:ASP:HB2	1.99	0.62
1:D:804:HIS:O	1:D:808:ILE:HG13	2.00	0.62
2:I:6:DA:H1'	2:I:7:DA:H5''	1.81	0.62
1:D:109:ARG:NH1	1:D:142:ILE:HD11	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:PHE:O	1:C:197:LEU:HD11	2.00	0.62
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.35	0.62
4:A:982:HOH:O	3:F:114:DA:H5'	2.00	0.62
3:L:104:DG:H2''	3:L:105:DC:H5'	1.81	0.62
1:C:117:VAL:HG22	1:C:133:ILE:HA	1.82	0.62
1:D:90:LEU:CD1	1:D:353:ILE:HG22	2.26	0.62
1:B:231:LYS:HG3	1:B:232:ASN:N	2.14	0.62
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.82	0.62
1:C:179:PRO:HB3	1:C:181:GLU:OE1	1.99	0.62
1:D:204:PHE:HE1	1:D:208:LYS:HD2	1.65	0.62
1:D:295:GLU:O	1:D:299:ASN:HA	2.00	0.62
1:D:365:TRP:HA	1:D:368:ILE:HD12	1.81	0.62
1:B:339:GLN:OE1	1:B:339:GLN:HA	2.00	0.61
1:C:116:GLU:HG2	1:C:324:ASN:OD1	2.00	0.61
1:C:356:GLN:NE2	1:C:356:GLN:H	1.98	0.61
1:D:269:SER:OG	1:D:355:ILE:HB	1.99	0.61
1:D:356:GLN:N	1:D:356:GLN:OE1	2.33	0.61
1:A:197:LEU:HD23	1:A:197:LEU:C	2.20	0.61
1:A:795:GLY:O	1:A:813:ARG:HD3	2.00	0.61
1:D:825:VAL:HG12	1:D:826:GLU:H	1.65	0.61
1:A:494:ARG:HD2	1:A:521:ASP:OD1	1.99	0.61
1:A:555:ALA:O	1:A:559:ARG:HG2	1.99	0.61
1:D:202:LEU:O	1:D:206:GLN:HG2	2.01	0.61
1:D:116:GLU:HB3	1:D:320:TYR:OH	2.00	0.61
1:D:455:SER:HA	1:D:675:ASN:O	2.00	0.61
1:D:485:HIS:HB3	1:D:556:GLN:HB2	1.82	0.61
1:C:313:ARG:HH11	1:C:313:ARG:HG3	1.66	0.61
1:A:365:TRP:CD2	1:A:566:LEU:HD23	2.36	0.61
1:B:856:ASP:HA	1:B:859:LYS:CB	2.31	0.61
1:D:542:LEU:HD12	1:D:545:ALA:HB3	1.81	0.61
1:C:464:TYR:HB3	1:C:466:ASP:OD2	2.00	0.61
1:A:314:GLU:CG	1:A:315:SER:H	2.14	0.61
1:A:540:GLU:O	1:A:544:ARG:HD3	2.01	0.61
1:B:696:LYS:O	1:B:756:GLY:HA2	2.00	0.61
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.81	0.61
1:D:439:LEU:O	1:D:443:ILE:HG13	2.01	0.61
1:B:824:VAL:HG13	1:B:830:VAL:HG11	1.81	0.61
1:C:129:ALA:HA	1:C:225:TYR:CZ	2.36	0.61
1:A:855:THR:OG1	1:A:857:LEU:HG	2.00	0.60
1:C:45:GLN:O	1:C:47:THR:HG23	2.01	0.60
1:D:500:LYS:CA	1:D:503:LEU:HB2	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:732:THR:HG22	1:D:745:LEU:HB3	1.83	0.60
1:D:812:ASN:CA	1:D:815:ILE:HG12	2.28	0.60
1:B:218:VAL:N	1:B:272:ASP:OD2	2.34	0.60
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.35	0.60
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.83	0.60
1:D:493:GLN:HA	1:D:549:GLU:OE1	2.01	0.60
1:D:461:MET:HE2	1:D:581:ARG:HH21	1.65	0.60
1:D:630:ASP:HB2	4:D:912:HOH:O	2.01	0.60
1:D:205:TRP:HE1	1:D:242:LEU:CA	2.14	0.60
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.84	0.60
3:F:111:DT:H2"	3:F:112:DT:H5"	1.83	0.60
1:A:481:GLN:HE21	1:A:559:ARG:NE	2.00	0.60
1:C:191:PHE:HD2	1:C:196:GLU:HG3	1.66	0.60
1:D:317:HIS:HA	1:D:320:TYR:HB3	1.82	0.60
1:D:511:ASP:OD2	1:D:533:LEU:HA	2.01	0.60
1:D:752:MET:CG	1:D:760:LEU:HD12	2.29	0.60
1:B:556:GLN:HG3	1:B:557:ILE:N	2.17	0.60
1:D:59:ARG:HG3	1:D:59:ARG:HH11	1.66	0.60
1:D:800:LYS:HE3	2:K:13:DG:H4'	1.84	0.60
2:G:16:DG:C2'	2:G:17:DC:H5"	2.32	0.60
1:A:97:TYR:O	1:A:352:LYS:NZ	2.34	0.60
1:A:85:MET:HE2	1:A:87:ASP:N	2.07	0.60
1:B:278:LYS:HE2	1:B:288:TYR:CD1	2.36	0.60
1:B:338:ARG:O	1:B:339:GLN:HB2	2.02	0.59
1:C:261:GLU:O	1:C:261:GLU:HG3	2.01	0.59
1:C:266:PHE:H	1:C:266:PHE:HD1	1.50	0.59
3:J:104:DG:C2'	3:J:105:DC:H5"	2.32	0.59
1:D:516:VAL:HG21	1:D:522:PHE:CE2	2.37	0.59
1:A:404:TYR:CD1	1:A:618:LEU:HD22	2.37	0.59
1:B:355:ILE:O	1:B:358:VAL:HG13	2.02	0.59
1:B:606:ASN:HD22	1:B:612:GLU:CA	2.13	0.59
1:A:792:ASP:HA	1:A:796:PHE:O	2.03	0.59
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.18	0.59
1:D:495:ASN:O	1:D:499:ILE:HG13	2.01	0.59
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.32	0.59
1:A:304:LYS:O	1:A:319:ARG:HD3	2.03	0.59
1:C:449:ARG:HH21	1:C:675:ASN:HB2	1.68	0.59
1:D:802:PRO:HG2	1:D:805:ILE:HG12	1.83	0.59
1:C:323:TYR:HD1	1:C:326:ILE:HD11	1.68	0.59
1:C:482:ARG:HH21	1:C:556:GLN:NE2	2.01	0.59
1:A:23:ASN:ND2	1:A:25:ARG:HH12	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:C	1:A:499:ILE:H	2.06	0.59
1:A:791:TYR:CD2	1:A:801:CYS:HA	2.37	0.59
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.68	0.59
1:B:771:PHE:HD1	1:B:774:LEU:HD12	1.68	0.59
1:D:152:LEU:HA	1:D:159:VAL:HG22	1.83	0.59
2:I:16:DG:H2''	2:I:17:DC:C5'	2.33	0.59
1:A:193:ASN:HB2	4:A:951:HOH:O	2.02	0.59
1:B:114:ASP:HB2	1:B:328:VAL:HG22	1.84	0.59
1:D:812:ASN:HA	1:D:815:ILE:CD1	2.33	0.59
1:B:229:ARG:NH2	1:B:233:ILE:HD11	2.18	0.59
1:D:113:PHE:HB3	1:D:138:HIS:ND1	2.18	0.59
1:D:433:THR:HG22	1:D:461:MET:HE3	1.85	0.59
1:B:154:SER:HB2	1:B:155:PRO:HD2	1.84	0.58
1:C:284:ASN:HD21	1:C:829:LYS:HZ1	1.49	0.58
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.02	0.58
1:A:338:ARG:HB3	1:A:340:PHE:CZ	2.38	0.58
1:C:277:TYR:O	1:C:281:SER:HB3	2.03	0.58
1:C:34:LYS:HG3	1:C:63:ALA:O	2.03	0.58
1:D:228:ASN:O	1:D:231:LYS:HG2	2.02	0.58
1:A:4:PHE:CE1	1:A:20:ILE:HB	2.38	0.58
1:B:305:TYR:HB2	1:B:312:LEU:HD22	1.85	0.58
1:C:284:ASN:HD21	1:C:829:LYS:NZ	2.00	0.58
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.85	0.58
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.83	0.58
1:C:878:LYS:HE3	4:I:205:HOH:O	2.03	0.58
1:A:516:VAL:CG1	1:A:526:ILE:HG21	2.34	0.58
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.14	0.58
1:B:815:ILE:CD1	1:B:855:THR:HG21	2.28	0.58
3:J:104:DG:C1'	3:J:105:DC:H5''	2.33	0.58
1:A:248:THR:HG22	1:A:265:LEU:HD23	1.85	0.58
1:A:525:GLU:O	1:A:529:LYS:HE3	2.04	0.58
1:C:11:ILE:HD13	1:C:247:LYS:HD3	1.85	0.58
1:D:474:GLU:HA	1:D:474:GLU:OE1	2.03	0.58
1:D:722:GLU:OE2	1:D:723:PRO:HD2	2.04	0.58
1:A:509:SER:O	1:A:534:SER:HB3	2.03	0.58
1:B:297:GLU:O	1:B:298:LEU:HD23	2.04	0.58
1:B:494:ARG:O	1:B:498:ILE:HG12	2.04	0.58
1:B:776:TYR:CB	1:B:863:LEU:HD13	2.32	0.58
1:C:514:LEU:HG	1:C:533:LEU:HD21	1.85	0.58
1:D:402:ASN:ND2	1:D:403:ARG:N	2.50	0.58
1:B:235:GLY:O	1:B:237:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:OD1	1:B:321:ILE:HG13	2.04	0.58
1:B:642:ARG:HB2	1:B:642:ARG:NH1	2.19	0.58
1:D:469:GLY:C	1:D:472:PRO:HD2	2.24	0.58
1:A:653:LYS:HD3	1:A:656:ARG:NH2	2.18	0.58
1:D:365:TRP:CD2	1:D:566:LEU:HD23	2.39	0.58
3:J:110:DA:H2''	3:J:111:DT:H5'	1.86	0.58
1:A:314:GLU:HG3	1:A:315:SER:H	1.68	0.57
1:B:197:LEU:HD23	1:B:197:LEU:C	2.24	0.57
1:B:387:PRO:HG2	1:B:389:GLN:NE2	2.12	0.57
1:B:747:GLU:HA	1:B:747:GLU:OE2	2.04	0.57
1:C:231:LYS:HG2	1:C:236:GLU:HA	1.85	0.57
1:D:160:GLU:HG3	1:D:161:GLU:N	2.19	0.57
1:D:732:THR:HG22	1:D:745:LEU:CB	2.34	0.57
1:B:133:ILE:HD12	1:B:133:ILE:N	2.18	0.57
1:C:291:ASP:O	1:C:295:GLU:HG2	2.03	0.57
1:C:355:ILE:O	1:C:358:VAL:HG13	2.04	0.57
1:A:489:MET:HB3	1:A:552:GLY:HA3	1.86	0.57
1:B:227:TYR:CD2	1:B:263:ILE:HD13	2.39	0.57
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.84	0.57
1:C:526:ILE:O	1:C:530:ILE:HG13	2.04	0.57
1:A:101:ILE:HG13	1:A:349:TYR:HB3	1.84	0.57
1:A:481:GLN:HE21	1:A:559:ARG:HE	1.52	0.57
1:C:78:ILE:CG1	1:C:80:LEU:HD23	2.34	0.57
1:D:105:HIS:O	1:D:107:LYS:N	2.37	0.57
1:D:289:SER:O	1:D:293:ILE:HG12	2.05	0.57
1:B:554:THR:CA	1:B:557:ILE:HG22	2.34	0.57
1:C:299:ASN:O	1:C:300:VAL:HG13	2.04	0.57
1:D:118:THR:HB	1:D:313:ARG:NE	2.16	0.57
1:C:227:TYR:HD2	1:C:228:ASN:ND2	2.02	0.57
2:E:15:DC:H2'	2:E:16:DG:C8	2.39	0.57
1:A:846:ILE:HG23	1:A:846:ILE:O	2.03	0.57
1:D:147:TYR:CE1	1:D:187:ILE:HD12	2.40	0.57
1:D:395:PHE:HD2	1:D:594:LEU:HD23	1.68	0.57
1:D:728:MET:HG2	3:L:113:DC:H5''	1.87	0.57
1:B:514:LEU:H	1:B:541:MET:CE	2.12	0.57
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.85	0.57
1:B:792:ASP:OD2	1:B:809:LEU:HD22	2.05	0.57
1:B:836:ARG:NH2	1:B:864:HIS:O	2.38	0.57
1:C:170:LEU:HD22	1:C:170:LEU:N	2.19	0.57
1:C:516:VAL:CG1	1:C:526:ILE:HD13	2.34	0.57
1:A:534:SER:O	1:A:538:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.85	0.57
1:B:298:LEU:HD13	1:B:333:GLN:HG2	1.86	0.57
1:B:441:ASP:CB	1:B:447:ALA:HB2	2.33	0.57
1:D:40:HIS:CE1	1:D:83:LEU:HD11	2.40	0.57
1:B:188:TYR:OH	1:B:190:PRO:HB3	2.05	0.57
1:C:249:ARG:HD3	1:C:251:LYS:HZ1	1.70	0.57
1:D:194:GLU:O	1:D:198:LEU:HD13	2.03	0.57
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.86	0.57
2:E:16:DG:H2''	2:E:17:DC:C5'	2.34	0.57
1:B:660:GLU:HB3	1:B:661:PRO:HD3	1.86	0.56
1:C:815:ILE:HG23	1:C:821:ALA:HB3	1.85	0.56
1:D:671:CYS:SG	1:D:679:HIS:HB2	2.45	0.56
1:B:204:PHE:CE1	1:B:208:LYS:HD2	2.40	0.56
1:B:523:SER:H	1:B:526:ILE:HD12	1.71	0.56
1:C:514:LEU:HD12	1:C:530:ILE:HG12	1.86	0.56
1:C:486:LYS:HD3	1:C:556:GLN:CD	2.26	0.56
1:C:71:TRP:O	1:C:75:MET:HG2	2.05	0.56
1:D:700:GLY:HA2	1:D:753:LEU:CD2	2.36	0.56
1:C:202:LEU:O	1:C:206:GLN:HG2	2.05	0.56
1:C:227:TYR:HD2	1:C:228:ASN:HD22	1.51	0.56
1:A:857:LEU:CD1	1:A:858:ILE:HG23	2.30	0.56
1:B:299:ASN:HD22	1:B:299:ASN:N	2.03	0.56
1:D:573:VAL:HG23	1:D:574:TRP:CD1	2.27	0.56
1:C:81:GLU:HG3	1:C:384:ARG:NH2	2.19	0.56
1:C:529:LYS:O	1:C:529:LYS:HG2	2.06	0.56
1:C:493:GLN:HA	1:C:549:GLU:OE1	2.05	0.56
1:C:658:ARG:HG2	1:C:658:ARG:HH11	1.70	0.56
1:D:679:HIS:O	1:D:680:LEU:HD23	2.05	0.56
1:D:44:SER:O	1:D:46:ALA:N	2.38	0.56
1:B:771:PHE:HA	1:B:774:LEU:HG	1.87	0.56
1:C:461:MET:CE	1:C:581:ARG:HB3	2.36	0.56
1:C:760:LEU:HD13	1:C:891:TYR:HA	1.86	0.56
1:D:513:PRO:HB3	1:D:541:MET:HB2	1.88	0.56
1:A:52:ILE:HD12	1:A:428:GLU:HB3	1.88	0.56
1:D:15:ILE:HD13	1:D:15:ILE:C	2.26	0.56
3:L:104:DG:H1'	3:L:105:DC:H5''	1.88	0.56
1:A:8:VAL:O	1:A:354:GLN:NE2	2.39	0.56
1:C:132:PRO:HB3	1:C:229:ARG:HH21	1.71	0.56
1:C:11:ILE:HD12	1:C:16:PHE:CD2	2.41	0.56
1:C:434:PHE:HE1	1:C:456:CYS:HB3	1.71	0.56
1:D:527:LYS:O	1:D:530:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:104:DG:H2''	3:F:105:DC:H5'	1.86	0.56
1:A:277:TYR:CE2	1:A:293:ILE:HD12	2.41	0.56
1:C:193:ASN:ND2	1:C:195:LYS:HB2	2.20	0.56
1:D:525:GLU:O	1:D:529:LYS:HG3	2.05	0.56
1:D:461:MET:HE1	1:D:581:ARG:HH21	1.69	0.56
1:D:761:GLN:NE2	1:D:893:LYS:HA	2.20	0.56
1:D:897:LEU:HD12	1:D:898:PHE:N	2.21	0.56
1:B:123:PHE:CD2	1:B:124:PRO:HD2	2.40	0.55
1:B:162:TRP:HZ3	1:B:188:TYR:HB2	1.70	0.55
1:D:243:SER:C	1:D:245:HIS:H	2.09	0.55
1:D:274:ILE:O	1:D:278:LYS:HG3	2.05	0.55
1:D:534:SER:O	1:D:538:LEU:HG	2.06	0.55
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.88	0.55
3:F:111:DT:C2'	3:F:112:DT:H5''	2.35	0.55
3:L:103:DG:H2''	3:L:104:DG:C8	2.41	0.55
1:A:202:LEU:O	1:A:206:GLN:HG2	2.06	0.55
1:A:687:ALA:HB2	1:A:715:MET:CE	2.35	0.55
1:B:121:ASP:OD1	1:B:122:GLY:N	2.32	0.55
1:C:125:GLU:O	1:C:128:GLN:HB2	2.06	0.55
1:C:314:GLU:O	1:C:315:SER:O	2.24	0.55
1:D:1:MET:HE3	1:D:102:LYS:HE3	1.87	0.55
3:F:104:DG:C1'	3:F:105:DC:H5''	2.33	0.55
1:C:477:LYS:O	1:C:481:GLN:HG3	2.06	0.55
1:C:728:MET:CE	3:J:113:DC:H3'	2.36	0.55
1:D:61:LEU:HD13	1:D:62:PHE:N	2.21	0.55
1:D:760:LEU:C	1:D:760:LEU:HD23	2.27	0.55
1:A:731:GLU:H	1:A:731:GLU:CD	2.09	0.55
1:B:220:SER:O	1:B:224:PRO:HG2	2.06	0.55
1:B:316:ASN:ND2	1:B:318:GLN:HB3	2.21	0.55
1:B:608:VAL:HG12	1:B:608:VAL:O	2.06	0.55
1:D:664:ASP:O	1:D:668:ARG:HG3	2.06	0.55
1:D:678:GLN:O	1:D:680:LEU:HG	2.06	0.55
1:A:170:LEU:HD12	1:A:173:GLN:HE21	1.72	0.55
1:A:649:ASP:O	1:A:653:LYS:HG2	2.07	0.55
1:B:316:ASN:HD21	1:B:319:ARG:H	1.53	0.55
1:B:542:LEU:O	1:B:546:GLN:HG3	2.07	0.55
1:C:176:ASP:HB2	1:C:178:VAL:HG23	1.88	0.55
1:C:109:ARG:HD2	1:C:209:THR:O	2.07	0.55
1:C:426:SER:OG	1:C:427:PRO:HD2	2.06	0.55
1:B:494:ARG:HD2	1:B:521:ASP:OD1	2.07	0.55
1:C:530:ILE:O	1:C:533:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:NH2	1:D:185:LYS:HG2	2.22	0.55
1:A:785:ALA:HB2	1:A:808:ILE:HD11	1.89	0.55
1:B:186:ILE:HG22	1:B:187:ILE:N	2.22	0.55
1:B:466:ASP:OD2	1:B:467:ARG:N	2.39	0.55
1:B:487:GLY:HA3	4:B:947:HOH:O	2.05	0.55
1:B:408:MET:CE	1:B:655:ALA:HB2	2.37	0.55
1:B:398:GLU:OE1	1:B:705:LYS:HE3	2.05	0.55
1:C:81:GLU:HG3	1:C:384:ARG:HH22	1.71	0.55
1:D:449:ARG:HH21	1:D:675:ASN:CB	2.16	0.55
1:D:118:THR:CB	1:D:313:ARG:HE	2.18	0.55
1:D:541:MET:O	1:D:544:ARG:HB2	2.07	0.55
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.89	0.55
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.88	0.55
1:D:725:LEU:HD11	1:D:750:ARG:HB2	1.88	0.55
1:B:316:ASN:C	1:B:316:ASN:HD22	2.10	0.54
1:B:330:ARG:O	1:B:333:GLN:HB3	2.07	0.54
1:D:248:THR:HA	1:D:266:PHE:CD1	2.42	0.54
1:B:554:THR:C	1:B:557:ILE:HG22	2.28	0.54
1:B:397:LYS:HB3	1:B:620:GLY:H	1.71	0.54
1:D:276:LEU:O	1:D:280:PHE:HD1	1.89	0.54
3:F:111:DT:H1'	3:F:112:DT:H5''	1.89	0.54
1:C:163:SER:OG	1:C:166:ILE:HG13	2.08	0.54
1:C:191:PHE:CE2	1:C:197:LEU:HA	2.43	0.54
1:D:6:LEU:HB2	1:D:18:ARG:O	2.08	0.54
3:F:104:DG:H2''	3:F:105:DC:C5'	2.37	0.54
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.88	0.54
1:D:160:GLU:H	1:D:317:HIS:CD2	2.24	0.54
1:D:819:ILE:O	1:D:819:ILE:HG12	2.07	0.54
1:D:823:GLN:HG2	1:D:824:VAL:O	2.08	0.54
1:A:365:TRP:CE2	1:A:566:LEU:HD23	2.42	0.54
1:A:848:TRP:CE2	1:A:854:ILE:HG12	2.42	0.54
1:B:516:VAL:HG11	1:B:526:ILE:HD11	1.89	0.54
1:C:526:ILE:HG22	1:C:530:ILE:HD11	1.89	0.54
1:D:205:TRP:HE1	1:D:242:LEU:C	2.10	0.54
1:D:273:TYR:OH	1:D:340:PHE:HB2	2.07	0.54
1:A:279:LYS:HG3	1:A:280:PHE:CE2	2.43	0.54
1:B:373:LEU:HB3	1:B:378:LYS:HB2	1.89	0.54
1:B:835:LEU:HD21	1:B:846:ILE:HG22	1.89	0.54
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.89	0.54
1:A:249:ARG:NH1	1:A:251:LYS:HE2	2.22	0.54
1:A:101:ILE:HD11	1:A:349:TYR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:LYS:HG2	1:D:898:PHE:CD2	2.43	0.54
1:C:365:TRP:CE2	1:C:566:LEU:HD23	2.43	0.54
1:C:516:VAL:HG21	1:C:522:PHE:CZ	2.43	0.54
1:D:700:GLY:HA2	1:D:753:LEU:HD22	1.89	0.54
1:D:809:LEU:HA	1:D:812:ASN:OD1	2.07	0.54
1:B:416:TYR:O	1:B:420:ILE:HG13	2.08	0.54
1:C:59:ARG:HH11	1:C:59:ARG:HG2	1.72	0.54
1:C:788:ILE:HG13	1:C:826:GLU:OE2	2.07	0.54
1:D:122:GLY:HA3	1:D:823:GLN:HE22	1.73	0.54
1:D:217:ASN:OD1	1:D:220:SER:HB2	2.08	0.54
1:D:594:LEU:O	1:D:597:ILE:HG22	2.08	0.54
1:D:87:ASP:OD1	1:D:363:LYS:HE3	2.08	0.54
1:D:888:LYS:C	1:D:889:LEU:HD12	2.29	0.54
1:A:493:GLN:O	1:A:496:GLY:N	2.41	0.54
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.37	0.54
1:B:809:LEU:O	1:B:813:ARG:HG3	2.08	0.54
1:C:214:THR:HG23	1:C:215:GLY:N	2.23	0.54
1:C:130:LYS:O	1:C:229:ARG:NH1	2.41	0.54
1:C:301:GLY:O	1:C:330:ARG:NH1	2.41	0.54
1:B:635:LYS:HG2	1:D:898:PHE:CE2	2.42	0.54
1:A:638:GLU:HB2	4:A:983:HOH:O	2.07	0.54
1:D:18:ARG:HA	1:D:27:ARG:O	2.08	0.54
1:D:450:PRO:HB2	1:D:456:CYS:SG	2.49	0.54
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.89	0.53
1:D:146:PHE:CD1	1:D:146:PHE:N	2.75	0.53
1:D:19:TYR:O	1:D:26:GLU:HA	2.08	0.53
1:D:25:ARG:NH1	1:D:25:ARG:HG3	2.23	0.53
1:B:120:PRO:HA	1:B:310:SER:HB3	1.90	0.53
1:A:127:SER:HA	1:A:228:ASN:ND2	2.24	0.53
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.38	0.53
1:B:115:ILE:HD11	1:B:133:ILE:HG13	1.87	0.53
1:B:163:SER:N	1:B:318:GLN:HE22	2.01	0.53
1:C:318:GLN:HE21	1:C:318:GLN:CA	2.19	0.53
1:D:204:PHE:CE1	1:D:208:LYS:HD2	2.44	0.53
3:H:105:DC:H2'	3:H:106:DT:H72	1.89	0.53
3:J:108:DT:H2''	3:J:109:DC:C5'	2.37	0.53
1:B:772:ARG:NH1	1:B:868:TYR:HB3	2.23	0.53
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.26	0.53
1:D:362:ILE:HG22	1:D:575:PHE:HD1	1.73	0.53
1:D:771:PHE:HA	1:D:774:LEU:HD12	1.91	0.53
1:A:602:ASN:ND2	1:A:616:PHE:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:VAL:CG1	1:B:830:VAL:HG11	2.39	0.53
1:D:481:GLN:O	1:D:485:HIS:HB2	2.09	0.53
1:D:50:PHE:HA	1:D:55:LYS:O	2.08	0.53
1:D:61:LEU:HD13	1:D:62:PHE:H	1.73	0.53
1:D:9:GLU:HB3	1:D:11:ILE:CD1	2.35	0.53
1:B:897:LEU:HD23	1:B:897:LEU:N	2.18	0.53
1:D:206:GLN:NE2	1:D:241:ARG:HB3	2.20	0.53
1:D:830:VAL:HG22	1:D:831:TYR:N	2.24	0.53
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.72	0.53
1:A:469:GLY:C	1:A:472:PRO:HD2	2.29	0.53
1:A:620:GLY:HA2	1:A:624:SER:O	2.08	0.53
1:B:198:LEU:O	1:B:200:GLU:N	2.42	0.53
1:B:764:PHE:O	1:B:768:GLU:HG3	2.08	0.53
1:B:835:LEU:HA	1:B:866:MET:HA	1.91	0.53
1:B:516:VAL:HG11	1:B:526:ILE:HD13	1.91	0.53
1:C:298:LEU:O	1:C:299:ASN:HB2	2.09	0.53
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.38	0.53
1:C:422:GLN:HG3	1:C:678:GLN:O	2.08	0.53
1:D:295:GLU:HG2	1:D:301:GLY:CA	2.28	0.53
1:A:280:PHE:N	1:A:280:PHE:CD2	2.74	0.52
1:B:273:TYR:CE2	1:B:335:ASP:HB2	2.44	0.52
3:J:104:DG:H2''	3:J:105:DC:H5'	1.90	0.52
1:B:194:GLU:C	1:B:196:GLU:H	2.12	0.52
1:B:700:GLY:HA2	1:B:753:LEU:HD22	1.89	0.52
1:D:150:ASP:OD1	1:D:321:ILE:HG13	2.10	0.52
1:D:516:VAL:HG21	1:D:522:PHE:HZ	1.72	0.52
1:A:301:GLY:O	1:A:330:ARG:NE	2.36	0.52
1:D:105:HIS:C	1:D:107:LYS:H	2.12	0.52
1:A:313:ARG:O	1:A:317:HIS:HB2	2.09	0.52
1:A:784:SER:HB3	1:A:829:LYS:HD3	1.91	0.52
1:B:502:ALA:CB	1:B:530:ILE:HG12	2.34	0.52
1:B:775:ASN:OD1	1:B:776:TYR:N	2.42	0.52
1:D:513:PRO:CB	1:D:541:MET:HB2	2.39	0.52
1:D:605:LEU:HA	1:D:608:VAL:HG22	1.91	0.52
3:J:101:DG:H2'	3:J:102:DC:C6	2.44	0.52
1:D:19:TYR:CE1	1:D:29:ARG:NE	2.73	0.52
1:B:226:VAL:O	1:B:230:ILE:HG13	2.10	0.52
1:B:334:ILE:CG1	1:B:338:ARG:HG3	2.40	0.52
1:B:340:PHE:O	1:B:343:LEU:HB3	2.09	0.52
1:C:511:ASP:OD2	1:C:533:LEU:HA	2.10	0.52
1:A:422:GLN:HG3	1:A:678:GLN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:24:GLY:CA	2.40	0.52
1:B:123:PHE:HE1	1:B:309:ILE:HD11	1.74	0.52
1:D:298:LEU:HB2	1:D:300:VAL:CG1	2.36	0.52
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.91	0.52
1:A:263:ILE:N	1:A:263:ILE:HD12	2.25	0.52
1:B:167:ALA:HB1	1:B:178:VAL:CG2	2.39	0.52
1:B:112:ASN:ND2	1:B:332:LEU:HD23	2.25	0.52
1:B:324:ASN:C	1:B:324:ASN:HD22	2.13	0.52
1:B:738:PRO:HB3	1:B:780:ALA:O	2.10	0.52
1:B:805:ILE:HD13	1:B:808:ILE:HD12	1.92	0.52
1:C:313:ARG:NH1	1:C:313:ARG:HG3	2.25	0.52
1:C:474:GLU:OE2	1:C:477:LYS:HD2	2.10	0.52
1:D:698:ILE:HG12	1:D:752:MET:O	2.09	0.52
1:A:731:GLU:HG3	1:A:879:PRO:CB	2.39	0.52
1:C:382:GLN:HB3	1:C:384:ARG:NH1	2.25	0.52
1:D:189:MET:HB3	1:D:191:PHE:CE1	2.45	0.52
1:D:399:PRO:HB3	1:D:619:TYR:HD2	1.74	0.52
1:A:290:LEU:O	1:A:294:SER:CB	2.57	0.51
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.31	0.51
1:B:660:GLU:CB	1:B:661:PRO:HD3	2.40	0.51
1:B:771:PHE:O	1:B:774:LEU:HG	2.10	0.51
1:B:854:ILE:HD11	1:B:858:ILE:CD1	2.40	0.51
1:C:134:ASP:O	1:C:135:ALA:HB2	2.10	0.51
1:C:154:SER:C	1:C:156:TYR:H	2.14	0.51
1:D:159:VAL:HB	1:D:317:HIS:CD2	2.45	0.51
1:B:731:GLU:HG3	1:B:879:PRO:HB3	1.92	0.51
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.40	0.51
1:D:298:LEU:HD11	1:D:333:GLN:HB3	1.91	0.51
1:B:162:TRP:CZ3	1:B:188:TYR:HB2	2.45	0.51
1:B:376:GLN:HB2	1:B:378:LYS:HG2	1.92	0.51
1:C:787:ASN:HB3	1:C:790:LYS:HB3	1.93	0.51
1:D:250:VAL:HG12	1:D:263:ILE:HD12	1.93	0.51
1:D:402:ASN:HD21	1:D:403:ARG:HG2	1.76	0.51
1:D:423:VAL:O	1:D:424:ASN:HB3	2.10	0.51
1:D:509:SER:H	1:D:534:SER:HB3	1.75	0.51
1:D:757:GLU:O	1:D:761:GLN:HG3	2.11	0.51
1:C:482:ARG:HG3	1:C:556:GLN:HG2	1.91	0.51
1:C:89:LYS:HE3	1:C:354:GLN:OE1	2.10	0.51
1:D:180:SER:O	1:D:183:ILE:HG22	2.10	0.51
1:D:189:MET:CE	1:D:200:GLU:HG2	2.41	0.51
2:E:8:DT:H2"	2:E:9:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:LYS:HE3	2:K:13:DG:C4'	2.40	0.51
1:A:401:PRO:O	1:A:402:ASN:HB2	2.11	0.51
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.92	0.51
1:A:687:ALA:HB2	1:A:715:MET:HE2	1.91	0.51
1:A:776:TYR:CD2	1:A:863:LEU:HD21	2.46	0.51
1:D:189:MET:HB3	1:D:191:PHE:HE1	1.76	0.51
1:D:251:LYS:HE2	1:D:264:THR:CG2	2.40	0.51
1:D:488:TYR:CE2	1:D:519:ARG:HD2	2.46	0.51
1:D:38:PHE:HE2	1:D:49:TYR:CG	2.29	0.51
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.75	0.51
1:D:849:PRO:HD2	4:D:918:HOH:O	2.11	0.51
1:D:31:VAL:HG21	1:D:92:TYR:OH	2.11	0.51
3:L:110:DA:H2''	3:L:111:DT:C5'	2.40	0.51
1:B:308:PRO:O	1:B:312:LEU:N	2.43	0.51
1:C:660:GLU:HB3	1:C:661:PRO:HD3	1.92	0.51
1:D:419:ILE:HD13	1:D:589:PHE:HD1	1.75	0.51
1:D:413:THR:OG1	1:D:682:PHE:HB2	2.10	0.51
3:J:104:DG:H2''	3:J:105:DC:H5''	1.92	0.51
3:J:111:DT:H2'	3:J:112:DT:H71	1.93	0.51
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.92	0.51
1:A:636:VAL:O	1:A:636:VAL:HG12	2.10	0.51
1:B:880:LEU:O	1:B:884:THR:HG23	2.09	0.51
1:C:121:ASP:HA	1:C:819:ILE:HG12	1.93	0.51
1:C:167:ALA:O	1:C:178:VAL:HB	2.11	0.51
1:C:323:TYR:CD1	1:C:326:ILE:HD11	2.46	0.51
1:A:481:GLN:HB3	1:A:559:ARG:HE	1.75	0.51
1:B:513:PRO:HG2	1:B:540:GLU:CG	2.41	0.51
1:B:824:VAL:HG13	1:B:830:VAL:CG1	2.40	0.51
1:D:859:LYS:CG	1:D:860:ASP:H	2.12	0.51
1:A:23:ASN:HD22	1:A:25:ARG:NH1	2.08	0.51
1:A:848:TRP:CD2	1:A:854:ILE:HG12	2.46	0.51
1:B:126:PRO:O	1:B:228:ASN:ND2	2.44	0.51
1:B:873:GLU:HA	1:B:877:ILE:HB	1.92	0.51
1:C:2:LYS:HE2	1:C:102:LYS:HB3	1.91	0.51
1:C:81:GLU:CD	1:C:384:ARG:HH12	2.14	0.51
1:D:777:ILE:HD11	1:D:853:GLU:OE1	2.11	0.51
2:I:16:DG:H2''	2:I:17:DC:H5'	1.92	0.51
1:A:730:LEU:HB3	1:A:883:PHE:CZ	2.46	0.51
1:A:9:GLU:HA	1:A:89:LYS:HD3	1.93	0.51
1:B:546:GLN:O	1:B:550:VAL:HG23	2.11	0.51
1:B:771:PHE:HE2	1:B:872:LEU:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.92	0.51
1:C:645:ASN:HD21	1:C:719:ARG:HH11	1.59	0.51
1:D:731:GLU:HG3	1:D:879:PRO:HB3	1.93	0.51
1:A:728:MET:CE	3:F:113:DC:H3'	2.41	0.50
1:B:134:ASP:OD2	1:B:320:TYR:HE2	1.94	0.50
1:D:305:TYR:CD2	1:D:312:LEU:HD22	2.46	0.50
1:A:492:ALA:HB1	1:A:549:GLU:HB2	1.92	0.50
1:A:664:ASP:O	1:A:668:ARG:HB2	2.10	0.50
1:B:326:ILE:HG23	1:B:330:ARG:HH21	1.76	0.50
1:C:83:LEU:CD1	1:C:83:LEU:N	2.74	0.50
1:D:248:THR:HA	1:D:266:PHE:HD1	1.76	0.50
1:D:530:ILE:HD11	1:D:541:MET:SD	2.51	0.50
1:A:654:PHE:O	1:A:658:ARG:HB2	2.12	0.50
1:B:282:PHE:O	1:B:283:THR:HG23	2.11	0.50
1:D:685:ARG:NH1	1:D:714:ASP:OD2	2.42	0.50
1:A:2:LYS:CD	1:A:2:LYS:H	1.93	0.50
1:A:553:MET:O	1:A:557:ILE:HG12	2.11	0.50
1:A:602:ASN:HD22	1:A:616:PHE:HB2	1.77	0.50
1:B:513:PRO:HG3	1:B:537:SER:O	2.12	0.50
1:D:118:THR:HG22	1:D:313:ARG:NH2	2.26	0.50
1:B:252:VAL:HG12	1:B:253:ILE:HG13	1.93	0.50
1:C:203:ASN:HD22	1:C:203:ASN:N	2.09	0.50
1:D:214:THR:OG1	1:D:215:GLY:N	2.44	0.50
1:D:40:HIS:HA	1:D:57:CYS:HB3	1.94	0.50
3:F:111:DT:H2''	3:F:112:DT:C5'	2.41	0.50
2:G:6:DA:H2''	2:G:7:DA:C5'	2.41	0.50
1:B:188:TYR:CD2	1:B:190:PRO:HD3	2.46	0.50
1:C:500:LYS:HE3	1:C:542:LEU:HD11	1.94	0.50
1:D:360:SER:CB	1:D:363:LYS:HB2	2.41	0.50
1:D:475:ILE:CD1	1:D:563:ILE:HG12	2.42	0.50
1:A:38:PHE:CD2	1:A:59:ARG:HA	2.47	0.50
1:B:298:LEU:O	1:B:299:ASN:HB2	2.11	0.50
1:C:310:SER:C	1:C:312:LEU:H	2.15	0.50
1:D:397:LYS:HB3	1:D:620:GLY:H	1.77	0.50
1:A:788:ILE:HD11	1:A:808:ILE:HG21	1.94	0.50
1:B:554:THR:O	1:B:557:ILE:HG22	2.11	0.50
1:C:426:SER:HB3	1:C:428:GLU:OE2	2.12	0.50
1:D:139:TYR:CG	1:D:140:ASP:N	2.80	0.50
1:D:308:PRO:CG	1:D:311:LYS:HB2	2.36	0.50
1:D:475:ILE:HD11	1:D:563:ILE:HG12	1.92	0.50
1:D:59:ARG:NH1	1:D:59:ARG:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:VAL:HG23	1:D:796:PHE:HB2	1.94	0.50
2:G:6:DA:H2"	2:G:7:DA:H5'	1.94	0.50
1:C:441:ASP:HB3	1:C:447:ALA:HB2	1.94	0.50
2:G:13:DG:H1	3:H:105:DC:N4	2.09	0.50
2:I:13:DG:H2"	2:I:14:DC:OP2	2.12	0.50
1:C:404:TYR:CD1	1:C:618:LEU:HD22	2.47	0.49
1:D:202:LEU:O	1:D:205:TRP:HB3	2.12	0.49
1:D:283:THR:HG23	1:D:285:GLN:HE22	1.76	0.49
1:D:317:HIS:HA	1:D:320:TYR:CB	2.42	0.49
1:A:202:LEU:CD1	1:A:242:LEU:HD13	2.42	0.49
1:A:281:SER:CB	1:A:338:ARG:HH21	2.22	0.49
1:A:849:PRO:HG2	4:A:933:HOH:O	2.12	0.49
1:C:189:MET:O	1:C:191:PHE:CE1	2.65	0.49
3:J:111:DT:C2'	3:J:112:DT:H71	2.42	0.49
1:B:12:GLY:CA	1:B:66:ARG:HH11	2.25	0.49
1:B:830:VAL:HA	1:B:850:SER:HB3	1.94	0.49
1:C:193:ASN:HD22	1:C:195:LYS:HB2	1.78	0.49
1:D:433:THR:N	1:D:462:MET:HE2	2.28	0.49
1:D:403:ARG:HH21	1:D:698:ILE:HG22	1.77	0.49
1:A:494:ARG:O	1:A:498:ILE:HG12	2.12	0.49
1:A:85:MET:HE3	1:A:85:MET:HA	1.94	0.49
1:D:229:ARG:NH1	1:D:233:ILE:HD11	2.26	0.49
1:D:300:VAL:O	1:D:300:VAL:HG13	2.12	0.49
1:D:305:TYR:HB2	1:D:312:LEU:HD13	1.94	0.49
1:A:508:LEU:N	1:A:508:LEU:HD12	2.28	0.49
1:B:167:ALA:HA	1:B:176:ASP:H	1.76	0.49
1:B:471:VAL:O	1:B:475:ILE:HG22	2.13	0.49
1:C:642:ARG:HH11	1:C:646:HIS:CD2	2.30	0.49
1:D:13:ASP:OD2	1:D:66:ARG:HB2	2.13	0.49
1:D:151:LEU:HD23	1:D:151:LEU:C	2.32	0.49
1:B:216:TRP:N	1:B:218:VAL:HG13	2.27	0.49
1:B:771:PHE:CD2	1:B:872:LEU:HD13	2.48	0.49
1:B:815:ILE:HG23	1:B:821:ALA:CB	2.43	0.49
1:B:822:PRO:HG2	1:B:855:THR:HB	1.93	0.49
1:C:245:HIS:O	1:C:246:ARG:C	2.51	0.49
1:D:656:ARG:O	1:D:661:PRO:HD3	2.12	0.49
2:G:16:DG:H2"	2:G:17:DC:H5'	1.93	0.49
1:B:755:GLU:HB3	1:B:759:SER:CB	2.43	0.49
1:D:512:GLU:CG	1:D:513:PRO:HD2	2.42	0.49
1:A:40:HIS:HD2	1:A:57:CYS:SG	2.36	0.49
1:B:133:ILE:CD1	1:B:229:ARG:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:CZ	1:B:309:ILE:HD11	2.48	0.49
1:B:738:PRO:HB3	1:B:780:ALA:N	2.27	0.49
1:C:347:MET:HE3	1:C:562:LEU:HD13	1.95	0.49
1:D:298:LEU:C	1:D:300:VAL:H	2.16	0.49
1:D:313:ARG:HD3	1:D:320:TYR:CZ	2.47	0.49
1:D:437:ALA:HB3	1:D:442:TYR:CZ	2.47	0.49
1:D:783:SER:O	1:D:830:VAL:N	2.44	0.49
1:A:170:LEU:HA	1:A:177:GLU:HG2	1.94	0.49
1:A:811:TYR:O	1:A:815:ILE:HG12	2.13	0.49
1:B:215:GLY:HA3	1:B:218:VAL:HG11	1.94	0.49
1:B:114:ASP:HB2	1:B:328:VAL:CG2	2.43	0.49
1:D:180:SER:HA	1:D:183:ILE:CG2	2.42	0.49
1:D:453:VAL:HG23	1:D:454:TYR:CE2	2.48	0.49
1:D:444:ASN:HA	1:D:599:ARG:NE	2.27	0.49
1:A:369:ILE:HG12	1:A:474:GLU:HG2	1.94	0.49
1:B:559:ARG:O	1:B:563:ILE:HG13	2.12	0.49
1:B:606:ASN:ND2	1:B:612:GLU:HA	2.19	0.49
1:B:655:ALA:HA	1:B:659:MET:HB2	1.94	0.49
1:C:13:ASP:HB3	1:C:64:ASN:HB2	1.93	0.49
1:C:481:GLN:HE21	1:C:559:ARG:NE	2.07	0.49
1:C:579:ASP:O	1:C:582:ASN:N	2.46	0.49
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.48	0.49
1:C:846:ILE:HG13	1:C:847:ALA:N	2.27	0.49
1:D:9:GLU:O	1:D:11:ILE:HG12	2.12	0.49
1:D:279:LYS:HB3	1:D:280:PHE:CE1	2.48	0.49
1:B:11:ILE:HD13	1:B:247:LYS:HG3	1.95	0.48
1:B:248:THR:HG22	1:B:265:LEU:HA	1.95	0.48
1:C:449:ARG:NH2	1:C:675:ASN:HB2	2.27	0.48
1:D:340:PHE:C	1:D:342:ASN:N	2.65	0.48
1:D:492:ALA:HB3	1:D:549:GLU:HA	1.95	0.48
1:A:436:VAL:HG12	1:A:437:ALA:O	2.13	0.48
1:B:822:PRO:HB2	1:B:849:PRO:HG2	1.96	0.48
1:C:13:ASP:OD2	1:C:64:ASN:HB2	2.12	0.48
1:D:268:ILE:HG22	1:D:269:SER:N	2.27	0.48
3:H:110:DA:H1'	3:H:111:DT:H5''	1.95	0.48
1:B:472:PRO:HA	1:B:475:ILE:HG22	1.95	0.48
1:D:112:ASN:HB3	1:D:214:THR:CG2	2.31	0.48
1:D:126:PRO:HA	1:D:225:TYR:HD1	1.77	0.48
1:D:230:ILE:HG23	1:D:234:PHE:HD2	1.79	0.48
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.96	0.48
1:A:454:TYR:HB3	1:A:463:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:VAL:CA	1:B:850:SER:HB3	2.43	0.48
1:C:109:ARG:CZ	1:C:142:ILE:HD12	2.43	0.48
1:D:305:TYR:O	1:D:307:GLY:N	2.46	0.48
3:J:113:DC:C2'	3:J:114:DA:H5''	2.36	0.48
1:B:159:VAL:HG11	1:B:313:ARG:HG2	1.95	0.48
1:B:38:PHE:CE2	1:B:59:ARG:HB2	2.48	0.48
1:C:130:LYS:CG	1:C:131:HIS:H	2.13	0.48
1:D:93:LEU:HD12	1:D:352:LYS:O	2.12	0.48
1:C:6:LEU:HD13	1:C:211:VAL:HG21	1.95	0.48
1:D:31:VAL:CG1	1:D:32:GLU:N	2.75	0.48
1:D:434:PHE:CZ	1:D:460:GLY:HA2	2.48	0.48
1:D:512:GLU:HG3	1:D:513:PRO:HD2	1.95	0.48
1:D:599:ARG:HH11	1:D:599:ARG:HG2	1.78	0.48
1:D:698:ILE:O	1:D:753:LEU:O	2.31	0.48
1:C:642:ARG:HD2	1:C:646:HIS:CE1	2.48	0.48
1:D:813:ARG:NH2	1:D:842:GLY:HA3	2.29	0.48
3:L:104:DG:H2''	3:L:105:DC:C5'	2.42	0.48
1:A:405:LYS:HG2	1:A:406:TYR:CE2	2.49	0.48
1:B:302:LYS:HG2	1:B:303:LEU:H	1.79	0.48
1:B:176:ASP:HA	1:B:319:ARG:HH21	1.78	0.48
1:B:456:CYS:SG	1:B:462:MET:HG2	2.53	0.48
1:C:170:LEU:HD22	1:C:170:LEU:H	1.79	0.48
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.49	0.48
1:C:51:ASP:HB2	4:C:919:HOH:O	2.14	0.48
1:D:31:VAL:CG1	1:D:32:GLU:H	2.23	0.48
1:D:368:ILE:HG22	1:D:474:GLU:OE2	2.12	0.48
1:D:512:GLU:CD	1:D:513:PRO:HD2	2.33	0.48
1:A:11:ILE:HD12	1:A:16:PHE:CD1	2.49	0.48
1:A:850:SER:O	1:A:852:THR:HG23	2.13	0.48
1:B:217:ASN:HB2	1:B:274:ILE:CD1	2.40	0.48
1:C:3:GLU:HG2	1:C:21:ASP:C	2.34	0.48
1:D:28:THR:HG22	1:D:29:ARG:N	2.29	0.48
1:D:596:TRP:CZ2	1:D:670:MET:HB2	2.48	0.48
1:D:81:GLU:CD	1:D:83:LEU:HD21	2.34	0.48
2:E:16:DG:H1'	2:E:17:DC:H5''	1.95	0.48
1:A:152:LEU:HB2	1:A:191:PHE:O	2.14	0.48
1:A:170:LEU:CG	1:A:173:GLN:HE21	2.26	0.48
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.49	0.48
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.48	0.48
1:A:752:MET:CG	1:A:760:LEU:HD22	2.43	0.48
1:A:86:ASP:OD1	1:A:86:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TYR:N	4:B:916:HOH:O	2.46	0.48
1:C:121:ASP:OD2	1:C:131:HIS:NE2	2.47	0.48
1:D:6:LEU:HD11	1:D:26:GLU:HG2	1.95	0.48
1:B:439:LEU:O	1:B:443:ILE:HG13	2.14	0.47
1:C:137:THR:OG1	1:C:324:ASN:ND2	2.47	0.47
1:C:508:LEU:HD23	1:C:508:LEU:C	2.35	0.47
1:C:455:SER:HA	1:C:675:ASN:O	2.13	0.47
1:D:205:TRP:CZ3	1:D:210:PRO:HG2	2.49	0.47
1:D:226:VAL:O	1:D:230:ILE:HG13	2.14	0.47
1:A:126:PRO:HB3	1:A:224:PRO:HB2	1.96	0.47
1:A:566:LEU:HD13	1:A:566:LEU:C	2.34	0.47
1:B:500:LYS:HA	1:B:503:LEU:HB2	1.95	0.47
1:B:708:TYR:CZ	1:B:728:MET:HG3	2.50	0.47
1:B:775:ASN:O	1:B:779:ILE:HG12	2.14	0.47
1:C:154:SER:C	1:C:156:TYR:N	2.66	0.47
1:C:496:GLY:O	1:C:500:LYS:HG2	2.14	0.47
1:D:687:ALA:HB2	1:D:715:MET:HE1	1.95	0.47
1:D:752:MET:HE1	1:D:884:THR:HA	1.96	0.47
1:B:191:PHE:CD2	1:B:197:LEU:HA	2.49	0.47
1:B:737:THR:CG2	1:B:738:PRO:HD2	2.45	0.47
1:C:11:ILE:CD1	1:C:247:LYS:HD3	2.43	0.47
1:C:343:LEU:HD11	1:C:558:ASN:ND2	2.30	0.47
1:D:151:LEU:HD21	1:D:154:SER:OG	2.14	0.47
3:H:103:DG:H2''	3:H:104:DG:OP2	2.14	0.47
1:A:206:GLN:NE2	1:A:246:ARG:HH22	2.11	0.47
1:A:303:LEU:HB3	1:A:323:TYR:HD1	1.80	0.47
1:C:313:ARG:O	1:C:317:HIS:HB2	2.15	0.47
1:C:439:LEU:HD11	1:C:592:MET:HB2	1.97	0.47
1:D:276:LEU:O	1:D:280:PHE:CD1	2.66	0.47
1:A:598:GLU:HG3	1:A:617:VAL:HG11	1.95	0.47
1:B:197:LEU:HD22	1:B:198:LEU:HD23	1.97	0.47
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.25	0.47
1:D:514:LEU:N	1:D:541:MET:HE2	2.28	0.47
1:D:411:ASP:HA	1:D:623:ASP:O	2.14	0.47
3:H:104:DG:H1'	3:H:105:DC:H5''	1.95	0.47
1:B:499:ILE:HA	1:B:530:ILE:HD11	1.95	0.47
1:C:111:ALA:HB2	1:C:210:PRO:HB3	1.96	0.47
1:C:176:ASP:O	1:C:178:VAL:N	2.41	0.47
1:C:330:ARG:O	1:C:334:ILE:HG13	2.15	0.47
1:C:818:ASN:HD22	1:C:821:ALA:N	2.11	0.47
1:D:7:THR:O	1:D:17:GLU:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:HIS:HD2	1:D:204:PHE:CE2	2.33	0.47
1:D:205:TRP:CD1	1:D:242:LEU:HA	2.49	0.47
1:D:244:PRO:HG2	1:D:267:GLY:HA3	1.97	0.47
1:D:40:HIS:HE1	1:D:83:LEU:HD11	1.80	0.47
1:D:516:VAL:CG1	1:D:526:ILE:HG21	2.30	0.47
2:E:16:DG:H2''	2:E:17:DC:H5'	1.96	0.47
1:A:481:GLN:NE2	1:A:559:ARG:NE	2.61	0.47
1:B:222:ALA:O	1:B:226:VAL:HG23	2.15	0.47
1:B:804:HIS:CE1	1:B:805:ILE:HG12	2.50	0.47
1:C:151:LEU:HD21	1:C:153:ASN:O	2.15	0.47
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.96	0.47
1:C:604:TYR:OH	1:C:658:ARG:HB3	2.15	0.47
1:C:818:ASN:HD21	1:C:820:ASP:HB2	1.80	0.47
1:D:527:LYS:C	1:D:530:ILE:HG22	2.34	0.47
2:G:17:DC:H2''	2:G:18:DG:O5'	2.15	0.47
3:J:101:DG:H2'	3:J:102:DC:C5	2.50	0.47
1:A:362:ILE:HG22	1:A:363:LYS:N	2.30	0.47
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.45	0.47
1:B:136:ILE:HD11	1:B:201:TYR:CE1	2.50	0.47
1:B:234:PHE:CD1	1:B:234:PHE:N	2.83	0.47
1:B:292:TYR:C	1:B:292:TYR:CD1	2.88	0.47
1:B:524:ASP:C	1:B:526:ILE:H	2.18	0.47
1:D:194:GLU:C	1:D:196:GLU:H	2.18	0.47
1:D:294:SER:O	1:D:296:PHE:N	2.47	0.47
1:D:28:THR:O	1:D:29:ARG:HB3	2.15	0.47
1:D:591:GLN:HG2	1:D:595:GLN:NE2	2.29	0.47
1:C:17:GLU:HG2	1:C:18:ARG:N	2.28	0.47
1:C:529:LYS:O	1:C:533:LEU:HD13	2.15	0.47
1:D:119:SER:OG	1:D:124:PRO:HD3	2.14	0.47
1:A:170:LEU:CD1	1:A:173:GLN:HE21	2.27	0.47
1:A:1:MET:HE3	1:A:24:GLY:HA3	1.97	0.47
1:A:360:SER:HB3	1:A:363:LYS:HB3	1.97	0.47
1:A:491:ALA:C	1:A:493:GLN:N	2.67	0.47
1:B:268:ILE:HG22	1:B:269:SER:N	2.30	0.47
1:B:159:VAL:HG11	1:B:313:ARG:CG	2.44	0.47
1:B:554:THR:HA	1:B:557:ILE:HG21	1.97	0.47
1:B:606:ASN:ND2	1:B:613:GLY:N	2.62	0.47
1:B:807:GLY:HA2	1:B:845:CYS:O	2.15	0.47
1:C:151:LEU:HD23	1:C:152:LEU:N	2.30	0.47
1:C:424:ASN:HD22	1:C:472:PRO:HG2	1.80	0.47
1:D:109:ARG:CZ	1:D:208:LYS:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ALA:HB1	1:D:139:TYR:O	2.15	0.47
1:D:162:TRP:HB3	1:D:188:TYR:CZ	2.50	0.47
1:D:4:PHE:CE2	1:D:20:ILE:HG21	2.49	0.47
1:D:642:ARG:HG3	1:D:642:ARG:HH11	1.80	0.47
1:A:148:VAL:HG21	1:A:325:ILE:HD11	1.97	0.47
1:A:154:SER:C	1:A:156:TYR:N	2.68	0.47
1:A:182:ILE:HG21	1:A:329:TYR:CE1	2.49	0.47
1:A:279:LYS:CG	1:A:280:PHE:CE2	2.97	0.47
1:A:285:GLN:HB3	1:A:292:TYR:HE2	1.79	0.47
1:A:403:ARG:HD2	1:A:887:ALA:O	2.15	0.47
1:A:414:SER:O	1:A:417:PRO:HD2	2.15	0.47
1:C:13:ASP:OD2	1:C:66:ARG:HB3	2.15	0.47
1:C:151:LEU:CD2	1:C:153:ASN:H	2.28	0.47
1:C:213:LEU:HD13	1:C:223:ILE:HD11	1.96	0.47
1:C:318:GLN:NE2	1:C:318:GLN:CA	2.78	0.47
1:D:506:PRO:O	1:D:508:LEU:HD22	2.14	0.47
1:D:286:PRO:O	1:D:829:LYS:HD2	2.14	0.47
1:A:787:ASN:HD22	1:A:790:LYS:HE2	1.78	0.46
1:B:725:LEU:HD22	1:B:753:LEU:HD12	1.96	0.46
1:C:154:SER:O	1:C:156:TYR:N	2.48	0.46
1:C:503:LEU:HG	1:C:538:LEU:HB3	1.97	0.46
1:C:578:TYR:OH	1:C:580:LEU:HB2	2.15	0.46
1:C:59:ARG:NH1	1:C:59:ARG:HG2	2.30	0.46
1:D:516:VAL:HG12	1:D:526:ILE:HD13	1.97	0.46
1:A:117:VAL:O	1:A:117:VAL:HG12	2.14	0.46
1:A:671:CYS:SG	1:A:676:ASN:HB2	2.55	0.46
1:B:198:LEU:O	1:B:199:MET:C	2.53	0.46
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.29	0.46
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.80	0.46
1:B:801:CYS:O	1:B:802:PRO:O	2.33	0.46
1:C:481:GLN:O	1:C:484:GLU:HB3	2.15	0.46
1:D:493:GLN:HA	1:D:549:GLU:CD	2.35	0.46
3:F:110:DA:H1'	3:F:111:DT:H5''	1.97	0.46
1:B:229:ARG:HE	1:B:233:ILE:HD11	1.78	0.46
1:B:755:GLU:HG2	1:B:759:SER:OG	2.15	0.46
1:C:530:ILE:HA	1:C:533:LEU:HD13	1.97	0.46
1:D:206:GLN:HE22	1:D:241:ARG:CB	2.22	0.46
1:D:345:LEU:HA	1:D:355:ILE:HD12	1.97	0.46
1:D:543:PHE:CA	1:D:546:GLN:HE21	2.08	0.46
3:H:107:DG:H2''	3:H:108:DT:OP2	2.14	0.46
1:B:499:ILE:HA	1:B:530:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:LEU:C	1:C:580:LEU:HD23	2.36	0.46
1:D:735:SER:O	1:D:782:VAL:HB	2.15	0.46
3:L:108:DT:H1'	3:L:109:DC:H5''	1.97	0.46
1:A:214:THR:HG21	1:A:341:ILE:HD11	1.97	0.46
1:B:150:ASP:OD2	1:B:151:LEU:N	2.49	0.46
1:B:458:PRO:HG3	1:B:592:MET:SD	2.56	0.46
1:B:489:MET:SD	1:B:553:MET:HG2	2.55	0.46
1:B:364:THR:HG21	1:B:562:LEU:HD11	1.97	0.46
1:C:450:PRO:HB2	1:C:456:CYS:SG	2.55	0.46
1:C:596:TRP:HZ2	1:C:669:GLU:HG2	1.80	0.46
1:D:143:ASP:HB3	1:D:147:TYR:OH	2.15	0.46
1:D:197:LEU:HD23	1:D:197:LEU:C	2.35	0.46
1:D:68:ALA:O	1:D:72:ILE:HG13	2.16	0.46
1:D:793:VAL:HG23	1:D:793:VAL:O	2.15	0.46
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.96	0.46
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.97	0.46
1:B:133:ILE:HD12	1:B:133:ILE:H	1.81	0.46
1:B:804:HIS:NE2	1:B:805:ILE:HG12	2.30	0.46
1:B:862:VAL:O	1:B:862:VAL:HG22	2.15	0.46
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.50	0.46
1:C:461:MET:HE2	1:C:581:ARG:HB3	1.96	0.46
1:D:347:MET:SD	1:D:562:LEU:HD11	2.56	0.46
1:D:747:GLU:O	1:D:751:ARG:HG3	2.15	0.46
1:A:6:LEU:HD11	1:A:20:ILE:CD1	2.46	0.46
1:A:261:GLU:C	1:A:262:ILE:HD12	2.34	0.46
1:A:426:SER:HB3	1:A:429:THR:HG23	1.98	0.46
1:A:470:VAL:O	1:A:474:GLU:HB2	2.15	0.46
1:A:492:ALA:CB	1:A:549:GLU:HB2	2.45	0.46
1:A:653:LYS:O	1:A:657:GLU:HG2	2.16	0.46
1:B:528:GLU:C	1:B:530:ILE:H	2.19	0.46
1:D:159:VAL:HB	1:D:317:HIS:CG	2.51	0.46
1:D:556:GLN:NE2	1:D:556:GLN:O	2.48	0.46
1:D:641:PHE:CG	1:D:647:TRP:HB3	2.51	0.46
1:D:799:PRO:O	1:D:800:LYS:HB2	2.16	0.46
1:D:833:LEU:HD22	1:D:866:MET:HE3	1.97	0.46
1:B:313:ARG:O	1:B:317:HIS:HB2	2.16	0.46
1:C:738:PRO:HG2	1:C:741:VAL:HB	1.98	0.46
1:C:818:ASN:ND2	1:C:821:ALA:H	2.11	0.46
2:G:12:DA:H61	3:H:106:DT:H3	1.64	0.46
1:A:482:ARG:CZ	1:A:556:GLN:HE21	2.28	0.46
1:B:115:ILE:CD1	1:B:133:ILE:HG12	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:O	1:B:299:ASN:HA	2.16	0.46
1:D:140:ASP:OD1	1:D:142:ILE:HG12	2.15	0.46
1:D:652:ASP:OD2	1:D:656:ARG:NH1	2.49	0.46
1:D:776:TYR:CD2	1:D:863:LEU:HD11	2.51	0.46
2:G:16:DG:H1'	2:G:17:DC:H5''	1.98	0.46
1:A:50:PHE:HD2	1:A:54:GLY:O	1.99	0.46
1:A:516:VAL:HG13	1:A:526:ILE:HG21	1.98	0.46
1:B:248:THR:HG22	1:B:265:LEU:HD23	1.97	0.46
1:C:170:LEU:HD12	1:C:177:GLU:OE2	2.16	0.46
1:D:630:ASP:O	1:D:632:ILE:N	2.49	0.46
2:I:4:CTG:H2''	2:I:5:DG:OP2	2.16	0.46
1:A:808:ILE:HD13	1:A:824:VAL:HG11	1.98	0.45
1:A:833:LEU:HD22	1:A:866:MET:HE3	1.98	0.45
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.97	0.45
1:B:808:ILE:HG23	1:B:824:VAL:HG21	1.98	0.45
1:B:834:PRO:O	1:B:866:MET:HA	2.16	0.45
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.46	0.45
1:C:482:ARG:HH21	1:C:556:GLN:HE22	1.63	0.45
1:D:137:THR:HG22	1:D:328:VAL:HG21	1.98	0.45
1:D:316:ASN:ND2	1:D:319:ARG:CB	2.78	0.45
2:I:16:DG:H2''	2:I:17:DC:H5''	1.98	0.45
1:A:420:ILE:HG12	1:A:586:ILE:HD11	1.99	0.45
1:B:815:ILE:HG23	1:B:821:ALA:HB3	1.98	0.45
1:D:344:SER:O	1:D:345:LEU:C	2.54	0.45
1:D:831:TYR:CD2	1:D:848:TRP:NE1	2.74	0.45
3:H:104:DG:H5''	4:H:161:HOH:O	2.15	0.45
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.51	0.45
1:A:788:ILE:CD1	1:A:808:ILE:HG21	2.46	0.45
1:B:200:GLU:O	1:B:204:PHE:N	2.46	0.45
1:C:426:SER:CB	1:C:428:GLU:OE2	2.65	0.45
1:C:647:TRP:CE3	1:C:651:LEU:HD12	2.51	0.45
1:D:344:SER:O	1:D:347:MET:N	2.49	0.45
1:D:351:ALA:HB3	1:D:353:ILE:HG12	1.98	0.45
1:D:38:PHE:CZ	1:D:59:ARG:HG2	2.51	0.45
1:D:687:ALA:HB2	1:D:715:MET:CE	2.46	0.45
1:D:789:ALA:O	1:D:792:ASP:HB3	2.17	0.45
1:D:813:ARG:HH22	1:D:843:ASP:H	1.64	0.45
3:H:104:DG:H2''	3:H:105:DC:H5'	1.96	0.45
1:B:391:TYR:HB2	1:B:392:PRO:HD2	1.99	0.45
1:C:286:PRO:HD2	1:C:292:TYR:CE1	2.51	0.45
1:C:451:SER:OG	1:C:452:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ILE:HG22	1:C:530:ILE:CD1	2.45	0.45
1:D:62:PHE:N	1:D:62:PHE:CD1	2.84	0.45
1:D:736:SER:HA	1:D:782:VAL:O	2.16	0.45
1:D:7:THR:HG21	1:D:18:ARG:HE	1.81	0.45
1:D:897:LEU:C	1:D:897:LEU:HD12	2.36	0.45
3:H:111:DT:H2"	3:H:112:DT:OP2	2.17	0.45
1:A:371:ASN:O	1:A:375:GLU:HG2	2.16	0.45
1:B:115:ILE:HG13	1:B:133:ILE:HG21	1.99	0.45
1:B:490:LEU:C	1:B:492:ALA:H	2.20	0.45
1:B:408:MET:SD	1:B:655:ALA:HB2	2.56	0.45
1:B:658:ARG:O	1:B:661:PRO:HD2	2.17	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.99	0.45
1:D:148:VAL:HG21	1:D:325:ILE:CD1	2.47	0.45
1:D:224:PRO:O	1:D:228:ASN:ND2	2.50	0.45
1:D:298:LEU:C	1:D:300:VAL:N	2.70	0.45
1:D:396:VAL:HG12	1:D:705:LYS:HD3	1.98	0.45
1:D:822:PRO:HB2	1:D:849:PRO:HG2	1.98	0.45
3:L:108:DT:C1'	3:L:109:DC:H5"	2.46	0.45
1:A:728:MET:HE2	3:F:113:DC:H3'	1.99	0.45
1:C:249:ARG:CD	1:C:251:LYS:HZ3	2.28	0.45
1:C:844:LYS:HZ1	2:I:12:DA:P	2.40	0.45
1:D:240:LYS:C	1:D:242:LEU:H	2.20	0.45
1:D:793:VAL:CG2	1:D:796:PHE:HB2	2.47	0.45
1:D:880:LEU:O	1:D:884:THR:HG23	2.17	0.45
1:A:491:ALA:C	1:A:493:GLN:H	2.20	0.45
1:B:333:GLN:O	1:B:336:ALA:HB3	2.15	0.45
1:C:116:GLU:HB3	1:C:320:TYR:OH	2.16	0.45
1:C:233:ILE:HG22	1:C:234:PHE:N	2.31	0.45
1:D:151:LEU:HD11	1:D:154:SER:OG	2.17	0.45
1:D:251:LYS:HE2	1:D:264:THR:HG21	1.97	0.45
3:J:105:DC:H2'	3:J:106:DT:H72	1.98	0.45
1:B:529:LYS:O	1:B:533:LEU:HG	2.15	0.45
1:C:153:ASN:HB2	1:C:192:ASP:O	2.17	0.45
1:C:231:LYS:C	1:C:233:ILE:H	2.20	0.45
1:C:300:VAL:HG23	1:C:300:VAL:O	2.17	0.45
1:C:685:ARG:HD2	1:C:685:ARG:C	2.37	0.45
1:D:285:GLN:HB3	1:D:292:TYR:CE2	2.52	0.45
1:D:365:TRP:O	1:D:369:ILE:HG13	2.17	0.45
1:D:367:ALA:O	1:D:370:PHE:HB3	2.16	0.45
1:D:395:PHE:CZ	1:D:397:LYS:HB2	2.52	0.45
1:D:800:LYS:H	2:K:13:DG:H5"	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:O	1:A:493:GLN:HB2	2.16	0.45
1:A:405:LYS:O	1:A:690:GLY:HA2	2.17	0.45
1:B:36:SER:O	1:B:37:LEU:HD13	2.17	0.45
1:C:234:PHE:HB3	1:C:238:THR:HG21	1.99	0.45
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.65	0.45
1:A:214:THR:OG1	1:A:215:GLY:N	2.50	0.45
1:B:134:ASP:OD2	1:B:320:TYR:CE2	2.70	0.45
1:B:312:LEU:HD23	1:B:320:TYR:HD1	1.81	0.45
1:B:606:ASN:ND2	1:B:612:GLU:CA	2.78	0.45
1:B:696:LYS:O	1:B:756:GLY:CA	2.64	0.45
1:B:751:ARG:CZ	1:B:763:TYR:HB2	2.47	0.45
1:D:212:ILE:HD13	1:D:269:SER:HB3	1.98	0.45
1:D:248:THR:CG2	1:D:249:ARG:N	2.79	0.45
1:D:114:ASP:HB3	1:D:328:VAL:HG12	1.98	0.45
1:D:484:GLU:C	1:D:486:LYS:N	2.70	0.45
1:D:7:THR:CG2	1:D:18:ARG:HG3	2.47	0.45
2:E:7:DA:H5'	4:E:19:HOH:O	2.16	0.45
2:G:12:DA:C2	3:H:107:DG:C2	3.05	0.45
2:K:9:DG:H2''	2:K:10:DA:OP2	2.15	0.45
2:K:15:DC:C2'	2:K:16:DG:C8	2.90	0.45
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.98	0.44
1:A:840:PRO:HD3	1:A:865:TRP:CE2	2.53	0.44
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.85	0.44
1:B:44:SER:C	1:B:46:ALA:H	2.20	0.44
1:B:685:ARG:HD2	1:B:685:ARG:C	2.38	0.44
1:B:898:PHE:C	1:B:900:MET:H	2.21	0.44
1:C:52:ILE:HG12	4:C:919:HOH:O	2.16	0.44
1:D:17:GLU:HG2	1:D:18:ARG:H	1.82	0.44
1:D:402:ASN:HD22	1:D:403:ARG:N	2.13	0.44
1:D:856:ASP:HA	1:D:859:LYS:HD2	1.99	0.44
2:K:13:DG:H2''	2:K:14:DC:OP2	2.17	0.44
1:A:189:MET:O	1:A:191:PHE:CE1	2.71	0.44
1:A:299:ASN:O	1:A:300:VAL:HG13	2.17	0.44
1:A:481:GLN:NE2	1:A:559:ARG:HE	2.14	0.44
1:B:1:MET:HE3	1:B:20:ILE:CG2	2.47	0.44
1:B:271:LEU:CD1	1:B:356:GLN:HA	2.46	0.44
1:B:502:ALA:HB3	1:B:530:ILE:CG1	2.39	0.44
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.52	0.44
1:B:808:ILE:O	1:B:808:ILE:HG22	2.16	0.44
1:B:831:TYR:CD2	1:B:850:SER:HA	2.51	0.44
1:C:405:LYS:O	1:C:690:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:MET:CE	1:C:581:ARG:HD2	2.34	0.44
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.88	0.44
1:D:137:THR:N	1:D:324:ASN:ND2	2.63	0.44
1:D:422:GLN:O	1:D:676:ASN:HB3	2.17	0.44
1:D:455:SER:OG	1:D:676:ASN:HA	2.16	0.44
1:D:514:LEU:HD12	1:D:530:ILE:HB	1.99	0.44
1:D:503:LEU:HG	1:D:538:LEU:HD13	1.99	0.44
1:A:745:LEU:HD13	1:A:876:PHE:HD1	1.82	0.44
1:B:775:ASN:HB3	1:B:778:SER:OG	2.17	0.44
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.32	0.44
1:C:274:ILE:HG23	1:C:275:ASP:N	2.32	0.44
1:C:426:SER:OG	1:C:428:GLU:OE2	2.34	0.44
1:C:520:PHE:O	1:C:521:ASP:C	2.55	0.44
1:A:227:TYR:CD2	1:A:263:ILE:HG12	2.52	0.44
1:B:114:ASP:HB3	1:B:324:ASN:HD21	1.83	0.44
1:C:12:GLY:C	1:C:14:SER:H	2.20	0.44
1:C:702:TRP:CZ3	1:C:710:LEU:HD21	2.53	0.44
1:D:340:PHE:C	1:D:342:ASN:H	2.19	0.44
1:D:497:GLU:O	1:D:498:ILE:HD13	2.18	0.44
1:D:459:ASN:OD1	1:D:584:THR:HG22	2.17	0.44
1:D:692:PRO:HG3	1:D:713:TRP:HZ2	1.82	0.44
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.33	0.44
1:D:788:ILE:HD11	1:D:825:VAL:O	2.17	0.44
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.99	0.44
1:B:608:VAL:HG11	1:D:897:LEU:HD21	2.00	0.44
1:B:800:LYS:HZ1	3:H:108:DT:H5"	1.83	0.44
1:C:178:VAL:CG2	1:C:322:SER:HB3	2.48	0.44
1:C:557:ILE:HD13	1:C:557:ILE:HA	1.84	0.44
1:D:294:SER:C	1:D:296:PHE:N	2.70	0.44
2:K:11:DC:H2"	2:K:12:DA:C8	2.52	0.44
1:A:154:SER:C	1:A:156:TYR:H	2.21	0.44
1:A:605:LEU:O	1:A:609:CYS:HB2	2.18	0.44
1:B:13:ASP:OD1	1:B:66:ARG:HB2	2.18	0.44
1:B:246:ARG:HH11	1:B:246:ARG:HG3	1.82	0.44
1:B:855:THR:HG23	1:B:858:ILE:HG12	2.00	0.44
1:C:197:LEU:C	1:C:197:LEU:HD23	2.37	0.44
1:C:530:ILE:HG23	1:C:533:LEU:HD22	2.00	0.44
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.99	0.44
3:H:109:DC:H2"	3:H:110:DA:O5'	2.16	0.44
1:A:777:ILE:HG23	1:A:831:TYR:CE2	2.53	0.44
1:B:188:TYR:CE2	1:B:190:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ILE:HD11	1:B:663:ILE:HG23	1.99	0.44
1:B:739:LYS:O	1:B:742:GLN:N	2.50	0.44
1:C:19:TYR:N	1:C:19:TYR:CD1	2.86	0.44
1:D:1:MET:O	1:D:2:LYS:O	2.35	0.44
1:D:575:PHE:O	1:D:577:TYR:N	2.51	0.44
1:D:578:TYR:OH	1:D:580:LEU:HD23	2.18	0.44
1:D:443:ILE:HD13	1:D:595:GLN:OE1	2.18	0.44
1:A:815:ILE:HG22	1:A:857:LEU:HD11	1.99	0.44
1:B:115:ILE:CG1	1:B:116:GLU:H	2.24	0.44
1:B:506:PRO:CB	1:B:535:ALA:HB2	2.48	0.44
1:B:555:ALA:O	1:B:559:ARG:HG2	2.18	0.44
1:B:481:GLN:NE2	1:B:559:ARG:NE	2.56	0.44
1:B:729:GLY:O	1:B:734:LYS:HE2	2.17	0.44
1:C:678:GLN:HG2	1:C:680:LEU:HG	1.99	0.44
1:D:830:VAL:CG2	1:D:831:TYR:N	2.81	0.44
3:H:104:DG:C1'	3:H:105:DC:H5''	2.47	0.44
1:A:546:GLN:O	1:A:547:ARG:C	2.56	0.44
1:B:425:ILE:HG23	1:B:463:TYR:CE2	2.53	0.44
1:B:658:ARG:C	1:B:661:PRO:HD2	2.39	0.44
1:C:148:VAL:HG11	1:C:325:ILE:HD11	1.99	0.44
1:D:137:THR:CG2	1:D:328:VAL:HG21	2.47	0.44
1:D:274:ILE:CG1	1:D:278:LYS:HE3	2.47	0.44
1:D:395:PHE:CE2	1:D:397:LYS:HB2	2.53	0.44
1:D:495:ASN:OD1	1:D:521:ASP:HA	2.18	0.44
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.53	0.44
1:A:21:ASP:C	1:A:21:ASP:OD2	2.57	0.43
1:A:362:ILE:HD11	1:A:569:ALA:HA	1.99	0.43
1:A:702:TRP:CD1	1:A:708:TYR:HB3	2.53	0.43
1:A:725:LEU:HD22	1:A:753:LEU:HD12	1.99	0.43
1:A:784:SER:HB3	1:A:829:LYS:NZ	2.33	0.43
1:B:115:ILE:CG1	1:B:116:GLU:N	2.77	0.43
1:B:180:SER:O	1:B:183:ILE:HG22	2.19	0.43
1:B:434:PHE:HD1	1:B:462:MET:HG3	1.83	0.43
1:B:582:ASN:O	1:B:586:ILE:HG13	2.18	0.43
1:C:523:SER:O	1:C:527:LYS:HG3	2.18	0.43
1:C:637:GLY:O	1:C:640:LYS:HB2	2.18	0.43
1:C:97:TYR:O	1:C:99:TYR:N	2.47	0.43
1:D:364:THR:HG22	1:D:365:TRP:N	2.33	0.43
1:D:421:ARG:NH1	1:D:479:PHE:CE2	2.84	0.43
3:J:105:DC:H2''	3:J:106:DT:C6	2.53	0.43
1:A:144:ASP:OD2	1:A:185:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HG3	1:B:21:ASP:HA	1.99	0.43
1:C:187:ILE:HG22	1:C:187:ILE:O	2.18	0.43
1:C:297:GLU:OE1	1:C:338:ARG:NH1	2.51	0.43
1:D:140:ASP:OD1	1:D:141:SER:N	2.51	0.43
1:D:248:THR:HG21	1:D:265:LEU:HD23	1.99	0.43
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.98	0.43
1:A:707:ARG:HA	1:A:728:MET:O	2.18	0.43
1:B:301:GLY:O	1:B:302:LYS:HB2	2.18	0.43
1:D:118:THR:HG21	1:D:313:ARG:HB3	2.00	0.43
1:D:143:ASP:C	1:D:145:ARG:N	2.72	0.43
1:D:23:ASN:HB2	1:D:24:GLY:H	1.57	0.43
1:D:340:PHE:O	1:D:342:ASN:N	2.51	0.43
1:D:437:ALA:HB3	1:D:442:TYR:CE2	2.53	0.43
1:D:725:LEU:HD11	1:D:750:ARG:CB	2.48	0.43
1:A:429:THR:HG21	1:A:469:GLY:CA	2.47	0.43
1:A:89:LYS:HB2	1:A:89:LYS:NZ	2.33	0.43
1:B:162:TRP:CH2	1:B:186:ILE:HG21	2.54	0.43
1:B:856:ASP:HA	1:B:859:LYS:HB2	2.00	0.43
1:C:20:ILE:CG2	1:C:24:GLY:HA2	2.49	0.43
1:C:510:VAL:HG12	1:C:510:VAL:O	2.18	0.43
1:D:151:LEU:HA	1:D:191:PHE:O	2.19	0.43
1:D:705:LYS:C	1:D:707:ARG:H	2.21	0.43
1:A:776:TYR:CG	1:A:863:LEU:HD21	2.53	0.43
1:A:796:PHE:CE1	1:A:813:ARG:HD2	2.53	0.43
1:B:191:PHE:CD1	1:B:197:LEU:HG	2.54	0.43
1:C:643:ASP:HB2	4:C:1005:HOH:O	2.17	0.43
1:D:270:VAL:O	1:D:271:LEU:HG	2.17	0.43
1:D:305:TYR:C	1:D:307:GLY:H	2.22	0.43
1:D:319:ARG:O	1:D:319:ARG:HD3	2.17	0.43
1:D:750:ARG:NH2	1:D:751:ARG:HG2	2.33	0.43
3:J:101:DG:C2'	3:J:102:DC:C6	3.01	0.43
1:C:180:SER:O	1:C:182:ILE:N	2.51	0.43
1:C:398:GLU:OE1	1:C:705:LYS:HE3	2.18	0.43
1:C:512:GLU:HB3	1:C:513:PRO:CD	2.48	0.43
1:C:458:PRO:HG2	1:C:592:MET:SD	2.58	0.43
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.53	0.43
1:D:486:LYS:O	1:D:490:LEU:HG	2.19	0.43
1:D:550:VAL:CA	1:D:553:MET:HB3	2.45	0.43
1:D:859:LYS:O	1:D:863:LEU:HD22	2.19	0.43
1:A:373:LEU:HD12	1:A:380:ILE:HG22	2.00	0.43
1:A:458:PRO:HG3	1:A:592:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HG2	1:A:482:ARG:HH11	1.84	0.43
1:B:316:ASN:ND2	1:B:316:ASN:C	2.71	0.43
1:B:6:LEU:HG	1:B:19:TYR:HA	1.99	0.43
1:C:811:TYR:HA	1:C:846:ILE:HD11	2.01	0.43
2:I:16:DG:C2'	2:I:17:DC:H5''	2.48	0.43
1:A:426:SER:OG	1:A:427:PRO:HD2	2.18	0.43
1:A:518:TYR:H	1:A:518:TYR:HD1	1.62	0.43
1:B:636:VAL:O	1:B:637:GLY:O	2.37	0.43
1:B:810:THR:CG2	1:B:841:PHE:HB3	2.49	0.43
1:D:673:TYR:C	1:D:675:ASN:H	2.20	0.43
1:D:405:LYS:O	1:D:699:GLY:HA3	2.18	0.43
1:D:811:TYR:HB2	1:D:846:ILE:HG13	2.01	0.43
1:D:881:GLU:O	1:D:882:GLY:C	2.57	0.43
1:A:304:LYS:HB2	1:A:304:LYS:HE3	1.69	0.43
1:A:385:SER:HB2	4:A:959:HOH:O	2.18	0.43
1:A:482:ARG:HD2	1:A:556:GLN:HG2	2.01	0.43
1:B:117:VAL:HB	1:B:124:PRO:HG3	2.01	0.43
1:B:771:PHE:HD1	1:B:774:LEU:CD1	2.30	0.43
1:B:799:PRO:O	1:B:800:LYS:C	2.57	0.43
1:B:897:LEU:H	1:B:897:LEU:CD2	2.22	0.43
1:C:136:ILE:O	1:C:148:VAL:HA	2.19	0.43
1:C:503:LEU:HD21	1:C:538:LEU:HB2	2.00	0.43
1:D:38:PHE:CE2	1:D:59:ARG:HG2	2.54	0.43
1:D:830:VAL:HG22	1:D:831:TYR:O	2.19	0.43
2:E:16:DG:C2'	2:E:17:DC:H5''	2.49	0.43
1:A:121:ASP:N	1:A:121:ASP:OD1	2.52	0.43
1:A:787:ASN:HB3	1:A:790:LYS:HE2	2.01	0.43
1:A:795:GLY:O	1:A:813:ARG:CD	2.67	0.43
1:A:873:GLU:HA	1:A:877:ILE:HB	2.00	0.43
1:B:159:VAL:HB	1:B:317:HIS:CG	2.54	0.43
1:B:178:VAL:O	1:B:179:PRO:C	2.57	0.43
1:B:45:GLN:O	1:B:47:THR:HG23	2.18	0.43
1:C:81:GLU:CG	1:C:384:ARG:HH22	2.32	0.43
1:D:295:GLU:CD	1:D:301:GLY:HA2	2.38	0.43
1:D:497:GLU:O	1:D:497:GLU:HG3	2.19	0.43
1:D:4:PHE:CZ	1:D:20:ILE:HD13	2.53	0.43
1:D:491:ALA:HA	1:D:521:ASP:OD1	2.19	0.43
1:D:83:LEU:HD22	1:D:381:PRO:HA	2.00	0.43
3:H:109:DC:H6	3:H:109:DC:H2'	1.72	0.43
2:I:6:DA:H2''	2:I:7:DA:C5'	2.47	0.43
1:B:738:PRO:HB2	1:B:778:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:ARG:HA	1:B:755:GLU:HB2	2.01	0.42
1:C:135:ALA:O	1:C:136:ILE:CG1	2.66	0.42
1:C:540:GLU:O	1:C:544:ARG:HD3	2.18	0.42
1:C:725:LEU:HD11	1:C:750:ARG:HB2	2.01	0.42
1:D:206:GLN:NE2	1:D:241:ARG:HD2	2.34	0.42
1:D:294:SER:OG	1:D:330:ARG:HG2	2.19	0.42
1:D:586:ILE:HG22	1:D:587:THR:N	2.34	0.42
1:D:770:GLU:O	1:D:774:LEU:HG	2.18	0.42
1:A:731:GLU:N	1:A:731:GLU:CD	2.71	0.42
1:A:752:MET:HG3	1:A:760:LEU:HD22	2.01	0.42
1:B:202:LEU:O	1:B:205:TRP:HB3	2.19	0.42
1:B:278:LYS:HG2	1:B:288:TYR:CE1	2.53	0.42
1:B:324:ASN:C	1:B:324:ASN:ND2	2.72	0.42
1:B:405:LYS:HG2	1:B:406:TYR:CD1	2.54	0.42
1:C:164:ILE:HG12	1:C:164:ILE:O	2.18	0.42
1:C:195:LYS:O	1:C:234:PHE:HZ	2.01	0.42
1:C:298:LEU:O	1:C:299:ASN:CB	2.67	0.42
1:D:131:HIS:C	1:D:229:ARG:HE	2.23	0.42
1:D:262:ILE:O	1:D:262:ILE:HG22	2.20	0.42
1:D:298:LEU:HD11	1:D:333:GLN:CB	2.49	0.42
3:L:110:DA:C2'	3:L:111:DT:H5''	2.49	0.42
1:A:347:MET:HE3	1:A:558:ASN:ND2	2.34	0.42
1:A:808:ILE:O	1:A:811:TYR:HB3	2.18	0.42
1:B:198:LEU:O	1:B:201:TYR:N	2.52	0.42
1:B:126:PRO:HB3	1:B:224:PRO:HB2	2.01	0.42
1:B:45:GLN:NE2	1:B:58:THR:OG1	2.53	0.42
1:B:745:LEU:O	1:B:749:ILE:HG13	2.19	0.42
1:B:771:PHE:CD1	1:B:774:LEU:HD12	2.51	0.42
1:B:772:ARG:NH1	1:B:868:TYR:CB	2.82	0.42
1:C:362:ILE:CD1	1:C:575:PHE:HB2	2.50	0.42
1:C:416:TYR:HB2	1:C:417:PRO:HD3	2.01	0.42
1:C:51:ASP:OD1	1:C:51:ASP:C	2.57	0.42
1:C:542:LEU:O	1:C:546:GLN:HG3	2.19	0.42
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.85	0.42
1:D:425:ILE:O	1:D:426:SER:HB2	2.19	0.42
1:D:449:ARG:O	1:D:450:PRO:C	2.58	0.42
1:D:496:GLY:HA2	1:D:499:ILE:HD12	2.01	0.42
1:D:579:ASP:C	1:D:579:ASP:OD2	2.57	0.42
1:D:747:GLU:HA	1:D:747:GLU:OE2	2.19	0.42
1:D:843:ASP:HB3	1:D:844:LYS:H	1.56	0.42
3:L:110:DA:C1'	3:L:111:DT:H5''	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ARG:HB2	1:A:581:ARG:NH1	2.34	0.42
1:A:738:PRO:HB3	1:A:780:ALA:O	2.19	0.42
1:B:240:LYS:C	1:B:242:LEU:H	2.23	0.42
1:B:513:PRO:HB3	1:B:541:MET:HE1	2.01	0.42
1:B:841:PHE:CZ	1:B:846:ILE:HD12	2.54	0.42
1:C:458:PRO:CG	1:C:592:MET:SD	3.07	0.42
1:C:516:VAL:HG12	1:C:526:ILE:HD13	2.01	0.42
1:C:85:MET:HA	1:C:380:ILE:HD11	2.02	0.42
1:A:439:LEU:O	1:A:443:ILE:HG13	2.19	0.42
1:A:523:SER:O	1:A:527:LYS:CB	2.68	0.42
1:B:218:VAL:HG23	1:B:219:GLU:N	2.33	0.42
1:B:299:ASN:N	1:B:299:ASN:ND2	2.66	0.42
1:B:494:ARG:HG3	1:B:495:ASN:ND2	2.35	0.42
1:C:180:SER:C	1:C:182:ILE:H	2.22	0.42
1:D:115:ILE:HA	1:D:135:ALA:O	2.20	0.42
1:D:405:LYS:O	1:D:690:GLY:HA2	2.19	0.42
1:D:481:GLN:CB	1:D:559:ARG:NE	2.69	0.42
1:D:51:ASP:C	1:D:51:ASP:OD2	2.58	0.42
1:D:805:ILE:HD13	1:D:808:ILE:HD12	2.01	0.42
3:H:109:DC:H1'	3:H:110:DA:H5'	2.01	0.42
1:A:83:LEU:HD12	1:A:83:LEU:N	2.35	0.42
1:A:861:ASP:O	1:A:864:HIS:HB3	2.19	0.42
1:B:176:ASP:OD2	1:B:318:GLN:HG3	2.19	0.42
1:B:671:CYS:SG	1:B:676:ASN:HB2	2.59	0.42
1:B:846:ILE:O	1:B:846:ILE:HG23	2.19	0.42
1:C:500:LYS:HE2	1:C:542:LEU:HD21	2.01	0.42
1:D:151:LEU:HG	1:D:192:ASP:O	2.18	0.42
1:D:25:ARG:CG	1:D:25:ARG:NH1	2.81	0.42
1:D:503:LEU:HG	1:D:538:LEU:HB3	2.01	0.42
1:D:403:ARG:NH2	1:D:698:ILE:HG22	2.33	0.42
1:D:873:GLU:HA	1:D:877:ILE:HB	2.02	0.42
1:D:761:GLN:HE22	1:D:893:LYS:HA	1.82	0.42
1:A:702:TRP:CZ3	1:A:710:LEU:HD21	2.54	0.42
1:A:725:LEU:HD11	1:A:750:ARG:HB2	2.02	0.42
1:B:202:LEU:CD1	1:B:242:LEU:HD13	2.50	0.42
1:B:228:ASN:O	1:B:231:LYS:HG2	2.20	0.42
1:B:475:ILE:HD13	1:B:566:LEU:HG	2.01	0.42
1:B:4:PHE:O	1:B:19:TYR:HB2	2.19	0.42
1:C:203:ASN:ND2	1:C:203:ASN:N	2.68	0.42
1:C:9:GLU:OE1	1:C:266:PHE:HA	2.19	0.42
1:C:266:PHE:CD1	1:C:266:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ILE:C	1:D:232:ASN:H	2.21	0.42
1:D:848:TRP:HB2	4:D:918:HOH:O	2.19	0.42
1:B:658:ARG:CD	1:D:897:LEU:HD22	2.46	0.42
2:E:6:DA:C1'	2:E:7:DA:H5''	2.45	0.42
2:K:16:DG:H5'	4:K:30:HOH:O	2.20	0.42
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.55	0.42
1:A:2:LYS:N	1:A:2:LYS:CD	2.68	0.42
1:A:408:MET:HE1	1:A:655:ALA:HB2	2.01	0.42
1:A:559:ARG:HA	1:A:562:LEU:HD23	2.01	0.42
1:B:315:SER:OG	1:B:316:ASN:N	2.52	0.42
1:B:48:LYS:O	1:B:377:ASN:HB3	2.20	0.42
1:B:732:THR:HG22	1:B:745:LEU:HB3	2.02	0.42
1:C:125:GLU:CD	1:C:126:PRO:HD2	2.40	0.42
1:D:219:GLU:HB3	1:D:272:ASP:OD2	2.19	0.42
1:D:247:LYS:O	1:D:266:PHE:HB2	2.20	0.42
1:D:289:SER:O	1:D:290:LEU:C	2.57	0.42
1:D:391:TYR:HB2	1:D:392:PRO:CD	2.34	0.42
1:D:743:LYS:HB2	1:D:743:LYS:HE3	1.90	0.42
2:E:10:DA:C2'	2:E:11:DC:C5'	2.95	0.42
1:A:395:PHE:HB2	1:A:591:GLN:CG	2.34	0.42
1:B:118:THR:HG23	1:B:118:THR:O	2.19	0.42
1:B:3:GLU:HG3	1:B:20:ILE:O	2.20	0.42
1:B:235:GLY:O	1:B:236:GLU:C	2.58	0.42
1:B:308:PRO:C	1:B:310:SER:N	2.73	0.42
1:B:365:TRP:CD2	1:B:566:LEU:HD23	2.55	0.42
1:B:709:ALA:HA	1:B:726:LYS:O	2.20	0.42
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.55	0.42
1:C:572:ASN:O	1:C:578:TYR:HB2	2.20	0.42
1:D:20:ILE:HD12	1:D:107:LYS:CB	2.50	0.42
1:D:285:GLN:C	1:D:287:SER:N	2.72	0.42
1:D:597:ILE:HD12	1:D:597:ILE:HA	1.82	0.42
1:D:599:ARG:HG2	1:D:599:ARG:NH1	2.34	0.42
1:D:614:GLU:HG2	1:D:631:LYS:HE3	2.02	0.42
1:D:7:THR:HG22	1:D:18:ARG:CB	2.48	0.42
3:F:113:DC:H2''	3:F:114:DA:OP2	2.18	0.42
3:L:110:DA:H2''	3:L:111:DT:H5'	2.02	0.42
1:B:426:SER:HB2	1:B:472:PRO:HD2	2.02	0.42
1:B:708:TYR:CE1	1:B:728:MET:HB2	2.55	0.42
1:C:178:VAL:O	1:C:179:PRO:O	2.38	0.42
1:C:3:GLU:HG2	1:C:21:ASP:CA	2.46	0.42
1:D:323:TYR:CE1	1:D:326:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:GLN:O	1:D:377:ASN:HB2	2.18	0.42
1:D:484:GLU:O	1:D:486:LYS:N	2.53	0.42
1:D:508:LEU:CD2	1:D:508:LEU:H	2.28	0.42
1:D:495:ASN:HD21	1:D:521:ASP:HA	1.85	0.42
1:D:708:TYR:CE1	1:D:728:MET:HB3	2.55	0.42
2:E:16:DG:H2''	2:E:17:DC:H5''	2.01	0.42
1:C:728:MET:HE2	3:J:113:DC:H3'	2.02	0.42
1:A:709:ALA:HA	1:A:726:LYS:O	2.20	0.41
1:B:480:ASN:O	1:B:483:LYS:HB2	2.20	0.41
1:B:662:ALA:HA	1:B:665:ARG:NH2	2.35	0.41
1:C:199:MET:HG2	1:C:234:PHE:CE2	2.55	0.41
1:C:303:LEU:HD21	1:C:319:ARG:CG	2.49	0.41
1:C:377:ASN:HA	1:C:377:ASN:HD22	1.68	0.41
1:D:7:THR:CG2	1:D:18:ARG:HE	2.32	0.41
1:D:319:ARG:HG2	1:D:319:ARG:NH1	2.33	0.41
1:D:351:ALA:O	1:D:352:LYS:HB2	2.19	0.41
1:D:685:ARG:HD2	1:D:685:ARG:C	2.40	0.41
3:F:103:DG:C2'	3:F:104:DG:H5'	2.49	0.41
3:L:106:DT:H2''	3:L:107:DG:OP2	2.20	0.41
1:D:729:GLY:N	3:L:113:DC:OP1	2.44	0.41
1:A:507:ASN:C	1:A:508:LEU:HD12	2.40	0.41
1:A:529:LYS:O	1:A:533:LEU:HD11	2.20	0.41
1:A:839:ASN:HA	1:A:840:PRO:HD3	1.77	0.41
1:B:231:LYS:HB2	1:B:231:LYS:HE3	1.83	0.41
1:B:738:PRO:HB3	1:B:780:ALA:C	2.40	0.41
1:B:737:THR:HG22	1:B:738:PRO:HD2	2.02	0.41
1:C:660:GLU:CB	1:C:661:PRO:CD	2.97	0.41
1:D:17:GLU:CG	1:D:18:ARG:N	2.82	0.41
1:D:273:TYR:O	1:D:273:TYR:HD1	2.03	0.41
1:D:423:VAL:O	1:D:424:ASN:CB	2.68	0.41
1:D:488:TYR:HE2	1:D:519:ARG:HD2	1.85	0.41
1:D:652:ASP:OD2	1:D:652:ASP:C	2.58	0.41
1:B:186:ILE:HG22	1:B:187:ILE:H	1.85	0.41
1:B:598:GLU:HG3	1:B:617:VAL:HG11	2.02	0.41
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.55	0.41
1:C:457:SER:O	1:C:459:ASN:N	2.53	0.41
1:D:144:ASP:O	1:D:145:ARG:NE	2.53	0.41
1:D:217:ASN:N	1:D:272:ASP:OD1	2.53	0.41
1:D:19:TYR:O	1:D:27:ARG:N	2.53	0.41
1:D:283:THR:HG21	1:D:285:GLN:HE22	1.83	0.41
1:D:830:VAL:CG2	1:D:847:ALA:HB1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:LYS:H	2:K:13:DG:C5'	2.33	0.41
1:C:162:TRP:CZ3	1:C:164:ILE:HB	2.55	0.41
1:C:167:ALA:O	1:C:176:ASP:O	2.38	0.41
1:C:189:MET:O	1:C:191:PHE:HE1	2.04	0.41
1:D:191:PHE:HD2	1:D:197:LEU:HA	1.83	0.41
1:D:285:GLN:HB3	1:D:292:TYR:HE2	1.86	0.41
1:D:449:ARG:HA	1:D:450:PRO:HD2	1.90	0.41
1:D:479:PHE:CD1	1:D:563:ILE:HD13	2.56	0.41
1:D:579:ASP:O	1:D:582:ASN:HB2	2.21	0.41
1:D:410:PHE:CD2	1:D:685:ARG:HA	2.56	0.41
2:E:6:DA:H2''	4:E:19:HOH:O	2.19	0.41
1:A:219:GLU:HG2	1:A:219:GLU:O	2.21	0.41
1:A:303:LEU:HD12	1:A:304:LYS:H	1.86	0.41
1:A:602:ASN:ND2	1:A:616:PHE:N	2.68	0.41
1:A:806:ARG:HD2	1:A:844:LYS:NZ	2.35	0.41
1:B:351:ALA:O	1:B:352:LYS:HB2	2.20	0.41
1:B:363:LYS:HD3	1:B:363:LYS:HA	1.84	0.41
1:B:395:PHE:HB2	1:B:591:GLN:CG	2.34	0.41
1:B:739:LYS:O	1:B:740:ALA:C	2.59	0.41
1:B:797:PRO:HB3	1:B:809:LEU:HD12	2.01	0.41
1:C:150:ASP:HB2	1:C:188:TYR:HE1	1.86	0.41
1:C:512:GLU:CB	1:C:513:PRO:HD2	2.48	0.41
1:C:514:LEU:CD1	1:C:530:ILE:HG12	2.51	0.41
1:D:110:VAL:HG11	1:D:341:ILE:HG21	2.03	0.41
1:D:243:SER:O	1:D:245:HIS:N	2.52	0.41
1:D:482:ARG:HB2	1:D:559:ARG:CB	2.36	0.41
1:D:543:PHE:HD1	1:D:546:GLN:HE22	1.67	0.41
1:D:582:ASN:O	1:D:585:ALA:N	2.54	0.41
1:A:154:SER:O	1:A:156:TYR:N	2.53	0.41
1:A:351:ALA:O	1:A:352:LYS:HB2	2.19	0.41
1:B:221:PHE:HE2	1:B:225:TYR:HD1	1.67	0.41
1:B:308:PRO:C	1:B:310:SER:H	2.24	0.41
1:B:678:GLN:O	1:B:680:LEU:HG	2.20	0.41
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.55	0.41
1:B:810:THR:HB	1:B:845:CYS:O	2.20	0.41
1:C:413:THR:O	1:C:414:SER:C	2.58	0.41
1:C:546:GLN:C	1:C:548:THR:N	2.74	0.41
1:C:591:GLN:HB2	1:C:591:GLN:HE21	1.66	0.41
1:D:65:MET:HB3	1:D:88:PHE:CE2	2.55	0.41
1:D:449:ARG:NH2	1:D:675:ASN:HB2	2.18	0.41
1:D:98:ASN:O	1:D:99:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HG22	1:A:530:ILE:CD1	2.45	0.41
1:B:302:LYS:HG2	1:B:303:LEU:N	2.36	0.41
1:B:343:LEU:HG	1:B:558:ASN:HD21	1.86	0.41
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.56	0.41
1:D:129:ALA:HA	1:D:225:TYR:HE1	1.84	0.41
1:D:415:LEU:O	1:D:419:ILE:HG13	2.21	0.41
1:D:421:ARG:HH11	1:D:421:ARG:HG3	1.86	0.41
1:D:544:ARG:HH11	1:D:544:ARG:HG3	1.85	0.41
1:A:395:PHE:CB	1:A:591:GLN:HG3	2.35	0.41
1:B:194:GLU:C	1:B:196:GLU:N	2.73	0.41
1:B:198:LEU:HD13	1:B:230:ILE:HG12	2.03	0.41
1:C:178:VAL:O	1:C:179:PRO:C	2.58	0.41
1:C:362:ILE:HD13	1:C:362:ILE:HA	1.90	0.41
1:C:37:LEU:HA	1:C:37:LEU:HD23	1.89	0.41
1:C:80:LEU:N	1:C:80:LEU:HD22	2.35	0.41
1:D:499:ILE:HB	1:D:542:LEU:HD13	2.03	0.41
1:D:812:ASN:C	1:D:815:ILE:HG12	2.41	0.41
3:F:111:DT:C1'	3:F:112:DT:H5''	2.50	0.41
2:G:13:DG:N2	3:H:105:DC:N3	2.60	0.41
1:A:37:LEU:HD11	1:A:72:ILE:HD11	2.03	0.41
1:B:365:TRP:CE2	1:B:566:LEU:HD23	2.55	0.41
1:C:151:LEU:CD2	1:C:152:LEU:N	2.84	0.41
1:D:136:ILE:HB	1:D:149:PHE:HB2	2.03	0.41
1:D:241:ARG:HA	1:D:241:ARG:HD3	1.95	0.41
1:D:465:LYS:HZ2	1:D:675:ASN:CG	2.24	0.41
1:D:586:ILE:O	1:D:589:PHE:N	2.54	0.41
1:D:81:GLU:HG2	1:D:83:LEU:CD2	2.51	0.41
1:D:830:VAL:HG23	1:D:848:TRP:C	2.41	0.41
2:I:7:DA:C8	2:I:8:DT:H72	2.56	0.41
1:A:655:ALA:HA	1:A:659:MET:HB2	2.03	0.41
1:B:198:LEU:C	1:B:200:GLU:N	2.74	0.41
1:B:707:ARG:NH1	1:B:729:GLY:O	2.54	0.41
1:B:846:ILE:HD11	1:B:858:ILE:CD1	2.25	0.41
1:C:274:ILE:CG2	1:C:275:ASP:N	2.83	0.41
1:D:14:SER:O	1:D:65:MET:HE1	2.21	0.41
1:D:380:ILE:HA	1:D:381:PRO:HD3	1.84	0.41
1:D:403:ARG:H	1:D:403:ARG:HG2	1.71	0.41
1:D:500:LYS:C	1:D:503:LEU:H	2.25	0.41
1:D:633:ILE:O	1:D:633:ILE:CG2	2.68	0.41
1:A:362:ILE:HD12	1:A:569:ALA:CA	2.48	0.41
1:A:38:PHE:CE2	1:A:59:ARG:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:O	1:A:424:ASN:HB3	2.21	0.41
1:A:48:LYS:HG2	4:A:957:HOH:O	2.19	0.41
1:A:661:PRO:O	1:A:665:ARG:HB2	2.21	0.41
1:B:496:GLY:O	1:B:542:LEU:HD13	2.21	0.41
1:B:606:ASN:ND2	1:B:613:GLY:H	2.19	0.41
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.56	0.41
1:C:2:LYS:HE2	1:C:102:LYS:CB	2.51	0.41
1:C:317:HIS:O	1:C:318:GLN:C	2.60	0.41
1:C:760:LEU:C	1:C:760:LEU:HD22	2.40	0.41
1:D:102:LYS:HB2	1:D:102:LYS:NZ	2.36	0.41
1:D:271:LEU:HD22	1:D:276:LEU:CD2	2.45	0.41
1:D:116:GLU:CB	1:D:320:TYR:OH	2.69	0.41
1:D:362:ILE:HG22	1:D:575:PHE:CD1	2.52	0.41
1:B:898:PHE:HE2	1:D:653:LYS:HZ2	1.62	0.41
1:D:793:VAL:C	1:D:795:GLY:H	2.24	0.41
2:G:15:DC:H2"	2:G:16:DG:H5'	2.01	0.41
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.56	0.40
1:A:283:THR:O	1:A:284:ASN:C	2.60	0.40
1:B:114:ASP:HB3	1:B:324:ASN:ND2	2.36	0.40
1:B:1:MET:CE	1:B:20:ILE:HG22	2.51	0.40
1:B:330:ARG:HA	1:B:333:GLN:HB2	2.03	0.40
1:B:329:TYR:CE2	1:B:333:GLN:NE2	2.89	0.40
1:B:690:GLY:O	1:B:711:ASN:HB3	2.21	0.40
1:B:781:SER:HB2	1:B:832:VAL:HB	2.03	0.40
1:C:176:ASP:C	1:C:178:VAL:H	2.23	0.40
1:D:189:MET:O	1:D:191:PHE:HD1	2.05	0.40
1:D:809:LEU:HD12	1:D:809:LEU:C	2.42	0.40
1:D:825:VAL:CG1	1:D:826:GLU:H	2.32	0.40
1:B:494:ARG:CG	1:B:495:ASN:ND2	2.84	0.40
1:B:491:ALA:HB3	1:B:519:ARG:O	2.21	0.40
1:C:353:ILE:HD12	1:C:357:SER:HB2	2.03	0.40
1:D:118:THR:O	1:D:313:ARG:NH2	2.53	0.40
1:D:183:ILE:HG23	1:D:184:ASP:N	2.36	0.40
1:D:223:ILE:CB	1:D:224:PRO:HD3	2.43	0.40
1:D:198:LEU:CD2	1:D:230:ILE:HG12	2.49	0.40
1:D:740:ALA:O	1:D:741:VAL:C	2.59	0.40
1:D:698:ILE:HG13	1:D:753:LEU:HD23	2.02	0.40
1:A:152:LEU:HD11	1:A:190:PRO:HB2	2.02	0.40
1:A:566:LEU:CD1	1:A:570:LEU:HD22	2.52	0.40
1:A:38:PHE:HE2	1:A:59:ARG:HB2	1.86	0.40
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:HIS:HE1	1:C:51:ASP:OD2	2.04	0.40
1:C:529:LYS:CG	1:C:529:LYS:O	2.69	0.40
1:C:605:LEU:HD13	1:C:616:PHE:CD2	2.56	0.40
1:D:516:VAL:CG1	1:D:526:ILE:HD13	2.52	0.40
1:D:692:PRO:HG3	1:D:713:TRP:CZ2	2.56	0.40
1:D:791:TYR:HB2	1:D:805:ILE:HG21	2.03	0.40
1:D:863:LEU:HD22	1:D:863:LEU:H	1.86	0.40
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.57	0.40
1:A:386:HIS:HB2	1:A:573:VAL:HB	2.04	0.40
1:A:636:VAL:O	1:A:636:VAL:CG1	2.69	0.40
1:B:108:ILE:O	1:B:110:VAL:HG23	2.21	0.40
1:B:1:MET:HE3	1:B:20:ILE:HG21	2.02	0.40
1:B:609:CYS:C	1:B:611:THR:N	2.74	0.40
1:C:218:VAL:HA	1:C:222:ALA:HB3	2.04	0.40
1:C:227:TYR:CD2	1:C:228:ASN:ND2	2.88	0.40
1:C:423:VAL:HB	1:C:425:ILE:HG13	2.03	0.40
1:C:13:ASP:CG	1:C:64:ASN:HB2	2.42	0.40
1:C:727:ILE:HD13	1:C:749:ILE:CD1	2.51	0.40
1:D:188:TYR:CG	1:D:189:MET:N	2.90	0.40
1:A:497:GLU:C	1:A:499:ILE:N	2.72	0.40
1:B:272:ASP:CG	1:B:274:ILE:HG22	2.42	0.40
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.89	0.40
1:B:589:PHE:C	1:B:589:PHE:CD1	2.94	0.40
1:C:250:VAL:HG23	1:C:261:GLU:OE2	2.21	0.40
1:D:198:LEU:N	1:D:198:LEU:HD12	2.37	0.40
1:D:217:ASN:OD1	1:D:217:ASN:O	2.40	0.40
1:D:272:ASP:HB3	1:D:274:ILE:HG22	2.03	0.40
1:D:319:ARG:HD3	1:D:323:TYR:CD1	2.56	0.40
1:D:535:ALA:O	1:D:539:ASN:ND2	2.54	0.40
1:D:681:MET:CE	1:D:681:MET:HA	2.52	0.40
1:D:811:TYR:C	1:D:813:ARG:N	2.74	0.40
1:D:837:GLU:HG2	1:D:837:GLU:H	1.71	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	890/906 (98%)	804 (90%)	74 (8%)	12 (1%)	12	26
1	B	893/906 (99%)	759 (85%)	107 (12%)	27 (3%)	4	9
1	C	886/906 (98%)	769 (87%)	94 (11%)	23 (3%)	5	12
1	D	886/906 (98%)	681 (77%)	162 (18%)	43 (5%)	2	3
All	All	3555/3624 (98%)	3013 (85%)	437 (12%)	105 (3%)	4	9

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
1	A	534	SER
1	B	121	ASP
1	B	236	GLU
1	B	306	ASP
1	B	534	SER
1	B	637	GLY
1	B	802	PRO
1	C	315	SER
1	D	2	LYS
1	D	21	ASP
1	D	23	ASN
1	D	106	THR
1	D	305	TYR
1	D	344	SER
1	D	611	THR
1	D	630	ASP
1	B	115	ILE
1	B	179	PRO
1	B	199	MET
1	B	304	LYS
1	B	509	SER
1	C	24	GLY
1	C	120	PRO
1	C	181	GLU
1	C	232	ASN
1	C	607	GLU
1	D	10	GLN

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Mol	Chain	Res	Type
1	D	29	ARG
1	D	45	GLN
1	D	129	ALA
1	D	295	GLU
1	D	306	ASP
1	D	508	LEU
1	D	576	ARG
1	D	631	LYS
1	D	656	ARG
1	D	843	ASP
1	A	99	TYR
1	A	843	ASP
1	B	272	ASP
1	B	537	SER
1	B	645	ASN
1	B	800	LYS
1	B	858	ILE
1	C	159	VAL
1	C	179	PRO
1	C	299	ASN
1	C	311	LYS
1	C	622	THR
1	D	24	GLY
1	D	169	LYS
1	D	291	ASP
1	D	405	LYS
1	D	450	PRO
1	D	521	ASP
1	D	622	THR
1	D	739	LYS
1	D	754	GLN
1	A	169	LYS
1	B	516	VAL
1	B	739	LYS
1	B	774	LEU
1	C	63	ALA
1	C	112	ASN
1	C	135	ALA
1	C	301	GLY
1	C	458	PRO
1	C	484	GLU
1	D	459	ASN

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Mol	Chain	Res	Type
1	D	579	ASP
1	D	850	SER
1	D	897	LEU
1	A	284	ASN
1	A	498	ILE
1	B	523	SER
1	C	98	ASN
1	C	177	GLU
1	C	300	VAL
1	C	511	ASP
1	D	44	SER
1	D	241	ARG
1	D	460	GLY
1	D	570	LEU
1	D	642	ARG
1	D	849	PRO
1	A	518	TYR
1	A	622	THR
1	A	637	GLY
1	B	45	GLN
1	B	286	PRO
1	B	505	ASN
1	B	636	VAL
1	C	430	ILE
1	D	270	VAL
1	C	124	PRO
1	B	187	ILE
1	D	157	GLY
1	D	470	VAL
1	D	795	GLY
1	A	799	PRO
1	B	120	PRO
1	A	499	ILE
1	B	729	GLY
1	D	729	GLY

### 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	785/803 (98%)	751 (96%)	34 (4%)	29	54
1	B	774/803 (96%)	737 (95%)	37 (5%)	25	49
1	C	780/803 (97%)	740 (95%)	40 (5%)	24	45
1	D	764/803 (95%)	722 (94%)	42 (6%)	21	41
All	All	3103/3212 (97%)	2950 (95%)	153 (5%)	25	47

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	22	SER
1	A	25	ARG
1	A	35	PRO
1	A	58	THR
1	A	100	GLU
1	A	101	ILE
1	A	128	GLN
1	A	134	ASP
1	A	154	SER
1	A	200	GLU
1	A	203	ASN
1	A	231	LYS
1	A	242	LEU
1	A	246	ARG
1	A	264	THR
1	A	284	ASN
1	A	342	ASN
1	A	358	VAL
1	A	384	ARG
1	A	403	ARG
1	A	466	ASP
1	A	474	GLU
1	A	479	PHE
1	A	544	ARG
1	A	581	ARG
1	A	668	ARG
1	A	718	THR
1	A	731	GLU
1	A	745	LEU
1	A	799	PRO

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Mol	Chain	Res	Type
1	A	816	LYS
1	A	855	THR
1	A	903	PHE
1	B	22	SER
1	B	28	THR
1	B	37	LEU
1	B	61	LEU
1	B	113	PHE
1	B	114	ASP
1	B	117	VAL
1	B	123	PHE
1	B	153	ASN
1	B	179	PRO
1	B	199	MET
1	B	203	ASN
1	B	225	TYR
1	B	234	PHE
1	B	261	GLU
1	B	273	TYR
1	B	303	LEU
1	B	316	ASN
1	B	324	ASN
1	B	334	ILE
1	B	337	LYS
1	B	338	ARG
1	B	428	GLU
1	B	479	PHE
1	B	497	GLU
1	B	541	MET
1	B	562	LEU
1	B	580	LEU
1	B	635	LYS
1	B	702	TRP
1	B	722	GLU
1	B	755	GLU
1	B	760	LEU
1	B	773	GLN
1	B	820	ASP
1	B	867	ASP
1	B	897	LEU
1	C	19	TYR
1	C	28	THR

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Mol	Chain	Res	Type
1	C	58	THR
1	C	90	LEU
1	C	102	LYS
1	C	105	HIS
1	C	128	GLN
1	C	132	PRO
1	C	148	VAL
1	C	151	LEU
1	C	213	LEU
1	C	217	ASN
1	C	219	GLU
1	C	231	LYS
1	C	273	TYR
1	C	281	SER
1	C	283	THR
1	C	284	ASN
1	C	306	ASP
1	C	318	GLN
1	C	342	ASN
1	C	356	GLN
1	C	411	ASP
1	C	424	ASN
1	C	428	GLU
1	C	436	VAL
1	C	440	HIS
1	C	456	CYS
1	C	475	ILE
1	C	479	PHE
1	C	562	LEU
1	C	591	GLN
1	C	642	ARG
1	C	660	GLU
1	C	702	TRP
1	C	731	GLU
1	C	760	LEU
1	C	860	ASP
1	C	873	GLU
1	C	898	PHE
1	D	4	PHE
1	D	9	GLU
1	D	15	ILE
1	D	19	TYR

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Mol	Chain	Res	Type
1	D	25	ARG
1	D	48	LYS
1	D	59	ARG
1	D	61	LEU
1	D	86	ASP
1	D	90	LEU
1	D	92	TYR
1	D	102	LYS
1	D	113	PHE
1	D	134	ASP
1	D	145	ARG
1	D	146	PHE
1	D	193	ASN
1	D	199	MET
1	D	206	GLN
1	D	272	ASP
1	D	282	PHE
1	D	323	TYR
1	D	362	ILE
1	D	363	LYS
1	D	391	TYR
1	D	402	ASN
1	D	428	GLU
1	D	459	ASN
1	D	474	GLU
1	D	475	ILE
1	D	485	HIS
1	D	524	ASP
1	D	557	ILE
1	D	580	LEU
1	D	633	ILE
1	D	646	HIS
1	D	649	ASP
1	D	686	GLU
1	D	702	TRP
1	D	755	GLU
1	D	769	LYS
1	D	828	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	23	ASN
1	A	40	HIS
1	A	45	GLN
1	A	98	ASN
1	A	173	GLN
1	A	206	GLN
1	A	217	ASN
1	A	284	ASN
1	A	356	GLN
1	A	371	ASN
1	A	377	ASN
1	A	422	GLN
1	A	481	GLN
1	A	485	HIS
1	A	493	GLN
1	A	507	ASN
1	A	546	GLN
1	A	556	GLN
1	A	558	ASN
1	A	602	ASN
1	A	678	GLN
1	A	787	ASN
1	A	812	ASN
1	A	864	HIS
1	B	45	GLN
1	B	112	ASN
1	B	173	GLN
1	B	203	ASN
1	B	284	ASN
1	B	299	ASN
1	B	316	ASN
1	B	318	GLN
1	B	324	ASN
1	B	376	GLN
1	B	389	GLN
1	B	481	GLN
1	B	558	ASN
1	B	606	ASN
1	B	645	ASN
1	B	812	ASN
1	B	818	ASN
1	C	10	GLN
1	C	40	HIS

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Mol	Chain	Res	Type
1	C	45	GLN
1	C	158	ASN
1	C	173	GLN
1	C	203	ASN
1	C	207	GLN
1	C	217	ASN
1	C	228	ASN
1	C	232	ASN
1	C	284	ASN
1	C	318	GLN
1	C	324	ASN
1	C	354	GLN
1	C	356	GLN
1	C	377	ASN
1	C	424	ASN
1	C	480	ASN
1	C	481	GLN
1	C	495	ASN
1	C	507	ASN
1	C	546	GLN
1	C	556	GLN
1	C	558	ASN
1	C	591	GLN
1	C	595	GLN
1	C	645	ASN
1	C	818	ASN
1	C	864	HIS
1	D	40	HIS
1	D	45	GLN
1	D	131	HIS
1	D	138	HIS
1	D	206	GLN
1	D	207	GLN
1	D	316	ASN
1	D	324	ASN
1	D	339	GLN
1	D	354	GLN
1	D	376	GLN
1	D	389	GLN
1	D	402	ASN
1	D	422	GLN
1	D	485	HIS

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Mol	Chain	Res	Type
1	D	504	HIS
1	D	546	GLN
1	D	556	GLN
1	D	558	ASN
1	D	591	GLN
1	D	606	ASN
1	D	646	HIS
1	D	675	ASN
1	D	676	ASN
1	D	679	HIS
1	D	773	GLN
1	D	823	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	CTG	I	4	3,2	19,23,24	0.97	2 (10%)	21,35,38	0.59	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTG	I	4	3,2	-	4/7/45/46	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C5-C4	2.91	1.55	1.52
2	I	4	CTG	C1'-N1	2.10	1.48	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	CTG	N3-C2-N1	-2.25	114.36	116.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	4	CTG	O4'-C1'-N1-C6
2	I	4	CTG	C2'-C1'-N1-C6
2	I	4	CTG	C2'-C1'-N1-C2
2	I	4	CTG	O4'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	CTG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	894/906 (98%)	-0.03	29 (3%) 47 41	21, 41, 114, 141	1 (0%)
1	B	897/906 (99%)	0.72	129 (14%) 2 1	26, 63, 157, 177	13 (1%)
1	C	890/906 (98%)	0.06	20 (2%) 62 57	19, 49, 103, 130	2 (0%)
1	D	890/906 (98%)	0.76	120 (13%) 3 2	62, 103, 147, 163	5 (0%)
2	E	14/18 (77%)	0.41	0 100 100	69, 87, 126, 130	0
2	G	13/18 (72%)	1.61	3 (23%) 0 0	59, 143, 168, 169	0
2	I	16/18 (88%)	-0.24	0 100 100	33, 45, 113, 113	0
2	K	12/18 (66%)	0.62	1 (8%) 11 6	41, 116, 144, 150	0
3	F	14/14 (100%)	0.12	0 100 100	87, 103, 120, 132	0
3	H	13/14 (92%)	1.06	1 (7%) 13 8	137, 149, 163, 168	0
3	J	14/14 (100%)	-0.18	0 100 100	35, 61, 89, 93	0
3	L	13/14 (92%)	0.77	0 100 100	119, 128, 134, 138	0
All	All	3680/3752 (98%)	0.38	303 (8%) 11 6	19, 63, 144, 177	21 (0%)

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	821	ALA	11.8
1	B	507	ASN	11.6
1	B	847	ALA	11.4
1	B	785	ALA	10.6
1	B	862	VAL	10.5
1	B	514	LEU	10.2
1	B	820	ASP	9.7
1	B	812	ASN	8.5
1	B	846	ILE	8.4
1	B	799	PRO	8.4
1	B	809	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	510	VAL	8.2
1	B	801	CYS	7.4
1	B	508	LEU	7.2
1	B	865	TRP	7.1
1	D	535	ALA	6.9
1	B	538	LEU	6.8
1	B	866	MET	6.6
1	B	819	ILE	6.6
1	B	786	ASN	6.4
1	B	851	GLY	6.4
1	B	861	ASP	6.3
1	B	798	GLY	6.3
1	B	503	LEU	6.2
1	B	535	ALA	6.1
1	D	819	ILE	6.1
1	B	496	GLY	6.0
1	B	850	SER	6.0
1	B	541	MET	5.9
1	D	523	SER	5.9
2	G	6	DA	5.8
1	D	170	LEU	5.7
1	B	818	ASN	5.7
1	B	815	ILE	5.7
1	D	286	PRO	5.7
1	B	863	LEU	5.6
1	D	393	GLY	5.6
1	B	822	PRO	5.6
1	B	811	TYR	5.5
1	B	857	LEU	5.5
1	D	850	SER	5.5
1	B	542	LEU	5.5
1	B	825	VAL	5.4
1	C	530	ILE	5.4
1	B	787	ASN	5.4
1	B	505	ASN	5.3
1	B	526	ILE	5.2
1	B	844	LYS	5.2
1	A	530	ILE	5.0
1	A	502	ALA	5.0
1	B	530	ILE	5.0
1	B	852	THR	5.0
1	B	516	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	816	LYS	5.0
1	B	782	VAL	4.9
1	D	179	PRO	4.9
1	A	508	LEU	4.9
1	D	395	PHE	4.9
1	D	145	ARG	4.9
1	B	849	PRO	4.8
1	B	509	SER	4.8
1	D	174	GLY	4.8
1	B	803	PHE	4.7
1	D	20	ILE	4.7
1	B	813	ARG	4.6
1	B	791	TYR	4.6
2	G	7	DA	4.5
1	D	507	ASN	4.4
1	B	827	GLY	4.4
1	D	394	ALA	4.4
1	B	845	CYS	4.4
1	A	498	ILE	4.3
1	B	793	VAL	4.3
1	D	779	ILE	4.3
1	C	500	LYS	4.3
1	D	514	LEU	4.2
1	B	802	PRO	4.2
1	D	180	SER	4.2
1	D	178	VAL	4.1
1	C	498	ILE	4.1
1	B	504	HIS	4.1
1	D	120	PRO	4.1
1	B	306	ASP	4.0
1	B	797	PRO	4.0
1	B	833	LEU	3.9
1	B	783	SER	3.9
1	B	539	ASN	3.8
1	D	504	HIS	3.8
1	D	784	SER	3.8
1	B	497	GLU	3.8
1	B	511	ASP	3.8
1	B	498	ILE	3.8
1	B	788	ILE	3.7
1	B	868	TYR	3.7
1	D	817	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	545	ALA	3.7
1	B	834	PRO	3.7
1	D	786	ASN	3.7
1	D	138	HIS	3.7
1	A	541	MET	3.6
1	A	497	GLU	3.6
1	B	506	PRO	3.6
1	D	339	GLN	3.6
1	D	513	PRO	3.6
1	B	848	TRP	3.6
1	A	499	ILE	3.6
1	B	499	ILE	3.6
1	D	192	ASP	3.6
1	D	1	MET	3.6
1	A	542	LEU	3.5
1	B	534	SER	3.5
1	D	522	PHE	3.5
1	B	790	LYS	3.5
1	D	793	VAL	3.5
1	B	525	GLU	3.5
1	D	548	THR	3.5
1	B	800	LYS	3.5
1	D	16	PHE	3.5
1	B	502	ALA	3.5
1	B	160	GLU	3.5
1	B	817	GLY	3.5
1	D	266	PHE	3.5
1	B	855	THR	3.4
1	C	495	ASN	3.4
1	B	513	PRO	3.4
1	B	523	SER	3.4
1	B	536	LYS	3.4
1	D	538	LEU	3.4
1	B	522	PHE	3.4
1	D	527	LYS	3.3
1	B	519	ARG	3.3
1	B	789	ALA	3.3
1	B	528	GLU	3.3
1	D	790	LYS	3.3
1	B	120	PRO	3.3
1	B	546	GLN	3.2
1	D	509	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	539	ASN	3.2
1	D	545	ALA	3.2
1	A	787	ASN	3.2
1	C	499	ILE	3.1
1	B	814	ALA	3.1
1	A	504	HIS	3.1
1	B	527	LYS	3.1
3	H	107	DG	3.1
1	D	147	TYR	3.1
1	D	265	LEU	3.1
1	D	782	VAL	3.0
1	A	500	LYS	3.0
1	D	517	ASP	3.0
1	D	811	TYR	3.0
1	D	849	PRO	3.0
1	B	780	ALA	2.9
1	B	175	GLY	2.9
1	C	532	LYS	2.9
1	D	282	PHE	2.9
1	D	117	VAL	2.9
1	D	298	LEU	2.9
1	B	305	TYR	2.9
1	D	792	ASP	2.9
1	D	162	TRP	2.9
1	A	505	ASN	2.9
1	D	184	ASP	2.9
1	B	842	GLY	2.9
1	B	781	SER	2.9
1	B	307	GLY	2.8
1	D	491	ALA	2.8
1	B	828	GLU	2.8
1	C	535	ALA	2.8
1	D	198	LEU	2.8
1	D	541	MET	2.8
2	K	7	DA	2.8
1	D	510	VAL	2.8
1	D	512	GLU	2.7
1	A	518	TYR	2.7
1	D	831	TYR	2.7
1	D	329	TYR	2.7
1	B	830	VAL	2.7
1	C	533	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	130	LYS	2.7
1	D	498	ILE	2.7
1	C	508	LEU	2.7
1	A	522	PHE	2.7
1	D	826	GLU	2.7
1	D	262	ILE	2.7
1	A	528	GLU	2.7
1	D	809	LEU	2.7
1	B	853	GLU	2.7
1	D	11	ILE	2.6
1	B	543	PHE	2.6
1	A	516	VAL	2.6
1	D	832	VAL	2.6
1	A	501	GLU	2.6
1	B	805	ILE	2.6
1	D	281	SER	2.6
1	C	541	MET	2.6
1	B	512	GLU	2.6
1	D	789	ALA	2.6
1	A	788	ILE	2.6
1	A	547	ARG	2.6
1	D	768	GLU	2.6
1	D	277	TYR	2.6
1	D	537	SER	2.6
1	D	194	GLU	2.5
1	B	518	TYR	2.5
1	D	783	SER	2.5
1	B	501	GLU	2.5
1	D	202	LEU	2.5
1	A	507	ASN	2.5
1	A	506	PRO	2.5
1	D	129	ALA	2.5
1	D	559	ARG	2.5
1	D	338	ARG	2.5
1	A	509	SER	2.5
1	D	519	ARG	2.5
1	B	810	THR	2.5
1	D	160	GLU	2.4
1	D	767	PHE	2.4
1	B	533	LEU	2.4
1	D	497	GLU	2.4
1	B	867	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	771	PHE	2.4
1	D	534	SER	2.4
1	D	166	ILE	2.4
1	D	542	LEU	2.4
1	B	831	TYR	2.4
1	D	787	ASN	2.4
1	D	152	LEU	2.4
1	B	126	PRO	2.4
1	D	488	TYR	2.4
1	B	172	GLU	2.3
1	D	175	GLY	2.3
1	D	546	GLN	2.3
1	C	301	GLY	2.3
1	A	510	VAL	2.3
1	B	858	ILE	2.3
2	G	10	DA	2.3
1	D	446	VAL	2.3
1	D	511	ASP	2.3
1	A	533	LEU	2.3
1	D	815	ILE	2.3
1	B	171	GLN	2.3
1	D	171	GLN	2.3
1	D	804	HIS	2.3
1	B	854	ILE	2.3
1	D	812	ASN	2.3
1	B	500	LYS	2.3
1	D	105	HIS	2.3
1	D	115	ILE	2.3
1	D	518	TYR	2.3
1	D	827	GLY	2.3
1	D	213	LEU	2.3
1	D	557	ILE	2.3
1	B	792	ASP	2.2
1	C	303	LEU	2.2
1	B	777	ILE	2.2
1	D	164	ILE	2.2
1	D	848	TRP	2.2
1	D	28	THR	2.2
1	D	119	SER	2.2
1	D	290	LEU	2.2
1	D	530	ILE	2.2
1	D	536	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	153	ASN	2.2
1	B	540	GLU	2.2
1	D	172	GLU	2.2
1	A	786	ASN	2.2
1	C	526	ILE	2.2
1	D	493	GLN	2.2
1	B	494	ARG	2.2
1	A	503	LEU	2.2
1	D	505	ASN	2.2
1	D	113	PHE	2.2
1	B	128	GLN	2.2
1	D	182	ILE	2.2
1	B	531	LYS	2.2
1	C	496	GLY	2.1
1	B	856	ASP	2.1
1	C	537	SER	2.1
1	A	809	LEU	2.1
1	B	774	LEU	2.1
1	D	133	ILE	2.1
1	D	203	ASN	2.1
1	D	245	HIS	2.1
1	B	123	PHE	2.1
1	C	502	ALA	2.1
1	A	493	GLN	2.1
1	B	806	ARG	2.1
1	C	503	LEU	2.1
1	C	514	LEU	2.1
1	B	517	ASP	2.1
1	B	524	ASP	2.1
1	C	513	PRO	2.1
1	B	393	GLY	2.1
1	D	132	PRO	2.1
1	C	504	HIS	2.0
1	B	127	SER	2.0
1	B	843	ASP	2.0
1	B	122	GLY	2.0
1	D	248	THR	2.0
1	D	520	PHE	2.0
1	A	536	LYS	2.0
1	D	506	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CTG	I	4	22/23	0.78	0.19	114,118,119,119	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.