



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:44 PM GMT

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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

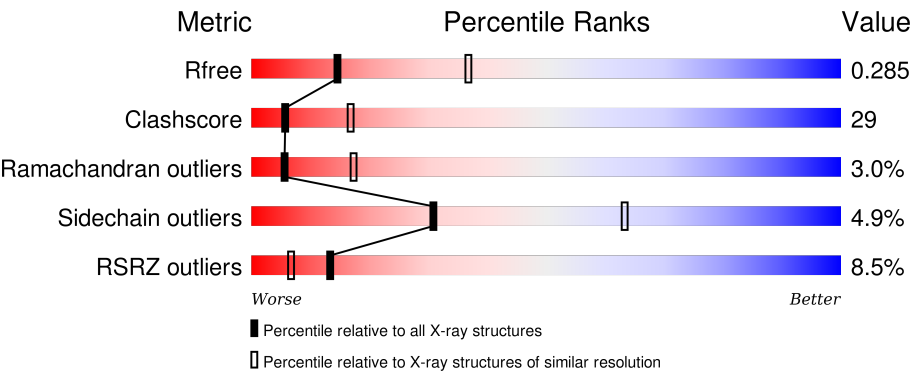
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 <sub>free</sub>	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	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>14%</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>

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Mol	Chain	Length	Quality of chain
2	G	18	<div><div><div></div><div></div><div></div></div><div>22%6%67%28%</div></div>
2	I	18	<div><div><div></div><div></div><div></div></div><div>39%50%6%6%</div></div>
2	K	18	<div><div><div></div><div></div><div></div></div><div>6%17%50%33%</div></div>
3	F	14	<div><div><div></div><div></div><div></div></div><div>29%71%</div></div>
3	H	14	<div><div><div></div><div></div><div></div></div><div>14%21%71%7%</div></div>
3	J	14	<div><div><div></div><div></div><div></div></div><div>14%86%</div></div>
3	L	14	<div><div><div></div><div></div><div></div></div><div>21%71%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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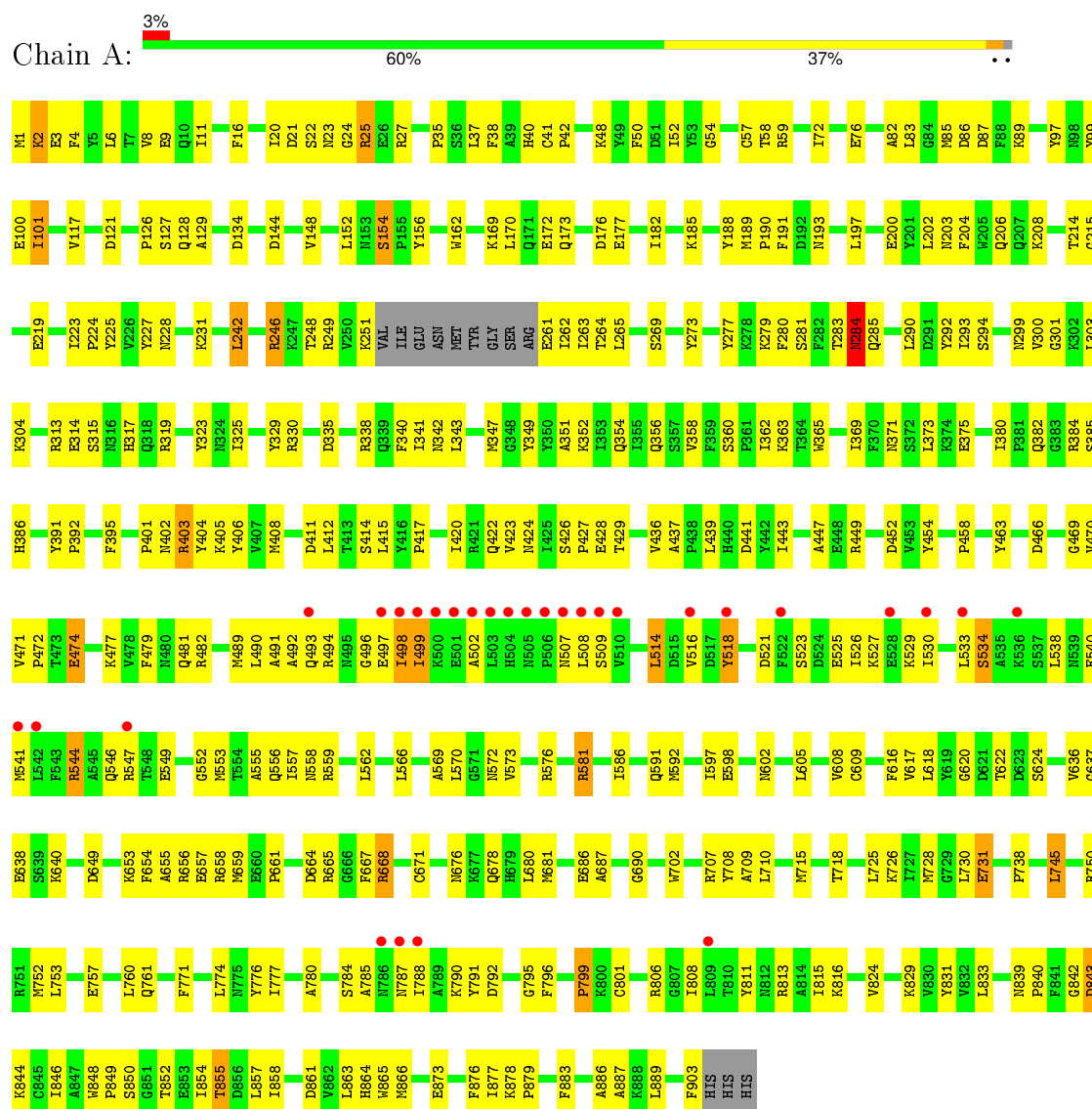
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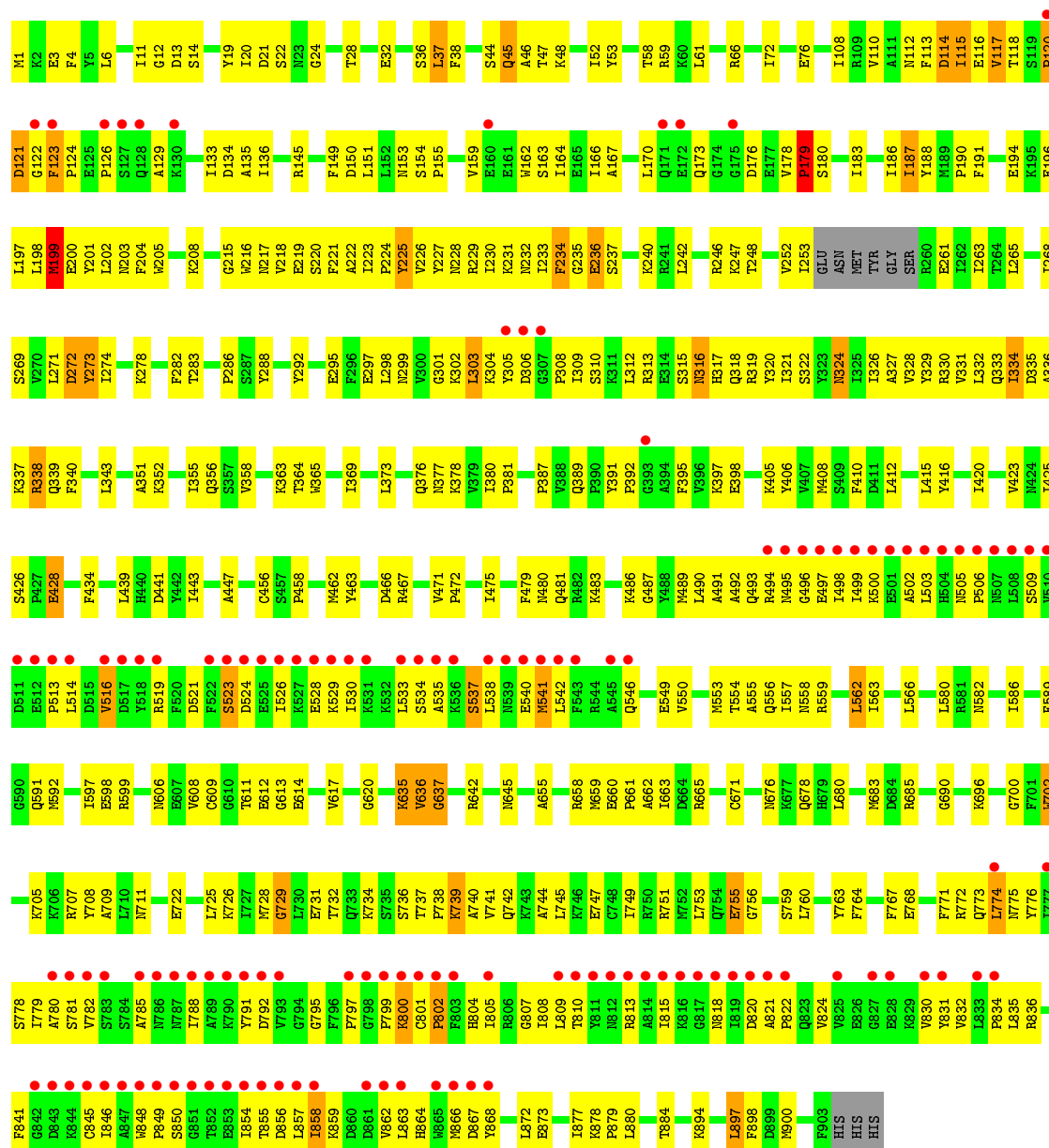
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	7	Total	O	0	0
			7	7		
4	J	6	Total	O	0	0
			6	6		
4	K	6	Total	O	0	0
			6	6		

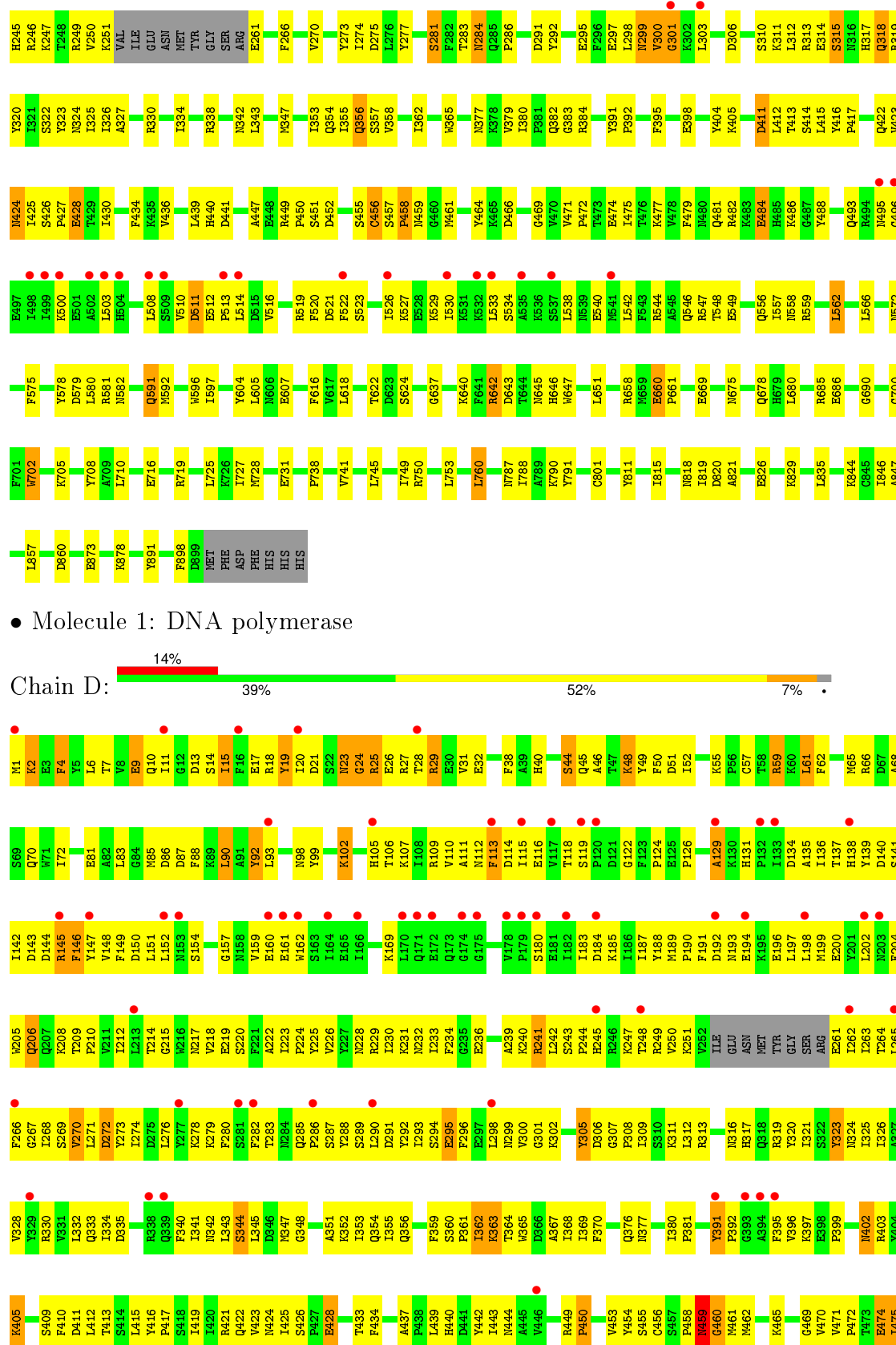
### 3 Residue-property plots

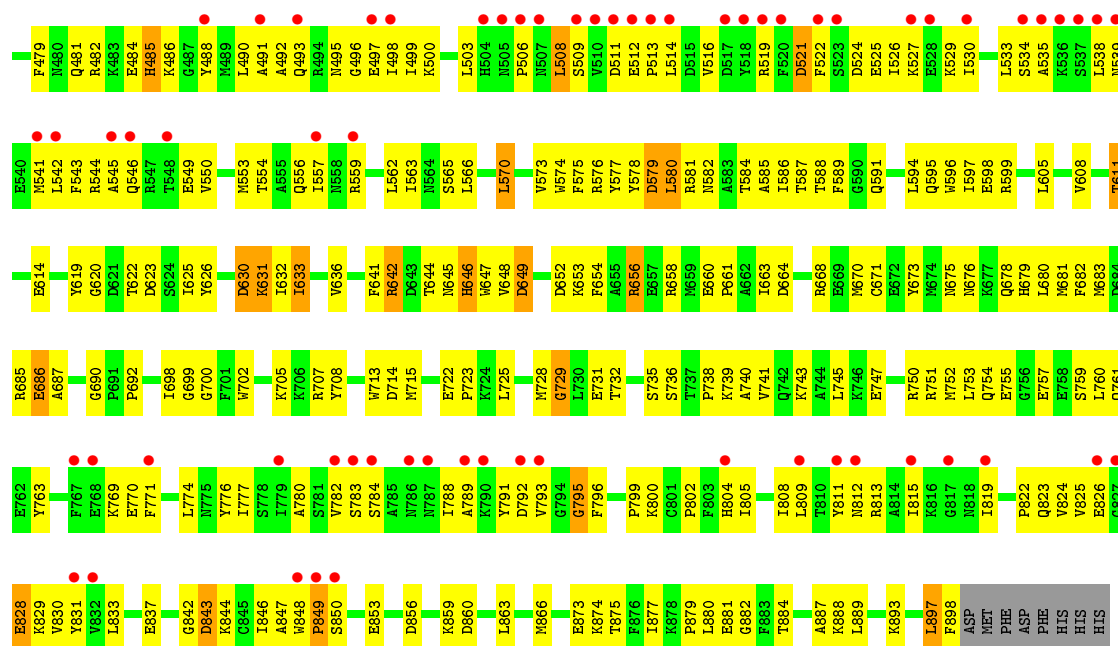
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: DNA polymerase



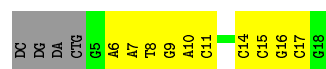






- Molecule 2: DNA (5'-D(\*CP\*GP\*AP\*(CTG)\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

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% 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%



- 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 K: 6% 17% 50% 33%



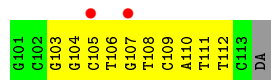
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*A)-3')

Chain F:  29% 71%



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

Chain H:  14% 21% 71% 7%




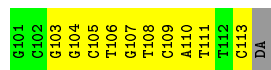
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*A)-3')

Chain J:  14% 86%



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

Chain L:  21% 71% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.70Å 123.00Å 163.94Å 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 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.275 0.229 , 0.285	Depositor DCC
$R_{free}$ test set	11700 reflections (9.63%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 243232 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:D:516:VAL:HG11	1:D:526:ILE:HG21	1.42	1.00
1:A:85:MET:HE2	1:A:87:ASP:H	1.23	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:D:112:ASN:HB3	1:D:214:THR:HG23	1.45	0.95
1:B:481:GLN:HE21	1:B:559:ARG:HE	1.08	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:D:573:VAL:HG23	1:D:574:TRP:HD1	1.35	0.92
1:B:514:LEU:H	1:B:541:MET:HE3	1.34	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:C:645:ASN:HD21	1:C:719:ARG:HD2	1.42	0.84
1:A:3:GLU:HG2	1:A:21:ASP:HA	1.60	0.84
1:B:897:LEU:H	1:B:897:LEU:HD23	1.41	0.83
1:A:449:ARG:HH12	1:A:452:ASP:HB3	1.42	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:D:271:LEU:HB3	1:D:276:LEU:HD11	1.60	0.80
1:B:493:GLN:HB3	1:B:549:GLU:OE2	1.81	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:395:PHE:HB2	1:D:591:GLN:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LYS:HE3	1:D:323:TYR:HE2	1.45	0.80
1:D:831:TYR:HD2	1:D:848:TRP:HE1	1.27	0.79
1:C:544:ARG:HG2	1:C:547:ARG:HH21	1.47	0.79
1:D:361:PRO:HB3	1:D:565:SER:HB2	1.65	0.79
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.63	0.79
1:C:249:ARG:HD3	1:C:251:LYS:NZ	1.96	0.79
2:K:16:DG:C2'	2:K:17:DC:H5''	2.13	0.79
1:C:382:GLN:HG2	1:C:383:GLY:N	1.98	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: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:434:PHE:CE1	1:D:460:GLY:HA2	2.18	0.79
1:B:115:ILE:HD11	1:B:133:ILE:HG12	1.65	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:D:516:VAL:HG21	1:D:522:PHE:CZ	2.20	0.77
1:C:219:GLU:HG3	1:C:270:VAL:HG11	1.66	0.77
1:B:115:ILE:HD11	1:B:133:ILE:CG1	2.15	0.77
1:A:249:ARG:HH11	1:A:251:LYS:HE2	1.49	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: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:A:283:THR:O	1:A:285:GLN:HG2	1.85	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:D:859:LYS:HG3	1:D:860:ASP:N	2.01	0.76
1:D:644:THR:O	1:D:648:VAL:HG23	1.86	0.76
1:B:776:TYR:HB3	1:B:863:LEU:HD13	1.68	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:C:303:LEU:HD23	1:C:323:TYR:HB2	1.69	0.74
1:B:322:SER:O	1:B:326:ILE:HG12	1.87	0.74
1:D:229:ARG:HG3	1:D:233:ILE:HD11	1.69	0.74
1:A:290:LEU:O	1:A:294:SER:HB2	1.86	0.74
1:B:115:ILE:HG12	1:B:116:GLU:N	2.01	0.74
1:A:502:ALA:O	1:A:538:LEU:HD13	1.87	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
2:K:10:DA:C2'	2:K:11:DC:H5''	2.17	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
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:C:78:ILE:HG13	1:C:80:LEU:HD23	1.70	0.73
1:B:658:ARG:HD2	1:D:897:LEU:HD22	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:D:85:MET:HE2	1:D:87:ASP:N	2.01	0.73
1:B:170:LEU:HB2	1:B:173:GLN:NE2	2.04	0.73
3:L:108:DT:H2''	3:L:109:DC:C5'	2.19	0.73
2:K:10:DA:H2''	2:K:11:DC:C5'	2.19	0.73
1:D:751:ARG:HD3	1:D:759:SER:OG	1.87	0.73
1:D:109:ARG:HD2	1:D:209:THR:O	1.88	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:449:ARG:NH1	1:A:452:ASP:HB3	2.04	0.72
3:H:104:DG:C2'	3:H:105:DC:H5''	2.19	0.72
1:A:428:GLU:N	1:A:428:GLU:OE1	2.22	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
1:A:362:ILE:HD12	1:A:569:ALA:HA	1.71	0.72
1:D:271:LEU:HD22	1:D:276:LEU:HD21	1.69	0.72
1:B:486:LYS:HG3	1:B:556:GLN:OE1	1.88	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:D:508:LEU:HD22	1:D:508:LEU:H	1.55	0.72
1:A:842:GLY:O	1:A:843:ASP:HB2	1.90	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:D:316:ASN:HD22	1:D:319:ARG:HB3	1.56	0.71
1:B:795:GLY:O	1:B:813:ARG:HD3	1.91	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
2:E:6:DA:H2''	2:E:7:DA:H5'	1.72	0.70
1:D:550:VAL:HA	1:D:553:MET:HB3	1.73	0.70
1:D:360:SER:HB2	1:D:363:LYS:HB2	1.73	0.70
1:D:229:ARG:O	1:D:233:ILE:HG13	1.90	0.70
1:C:815:ILE:HD12	1:C:821:ALA:CB	2.21	0.70
1:A:206:GLN:HE22	1:A:246:ARG:HH22	1.39	0.70
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.56	0.70
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.26	0.70
2:G:16:DG:H2''	2:G:17:DC:C5'	2.22	0.70
1:B:1:MET:HE1	1:B:24:GLY:HA2	1.73	0.70
1:D:422:GLN:NE2	1:D:681:MET:HG2	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:HG13	1:B:338:ARG:HG3	1.73	0.70
1:A:422:GLN:NE2	1:A:680:LEU:H	1.89	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:B:136:ILE:CG2	1:B:149:PHE:HB2	2.19	0.69
1:C:645:ASN:ND2	1:C:719:ARG:HD2	2.08	0.69
1:D:198:LEU:HD23	1:D:230:ILE:HG12	1.75	0.69
1:B:554:THR:HA	1:B:557:ILE:HG22	1.75	0.69
1:D:305:TYR:CG	1:D:312:LEU:HD22	2.27	0.69
1:A:224:PRO:HA	1:A:263:ILE:HD13	1.75	0.69
1:D:191:PHE:CZ	1:D:200:GLU:HB3	2.27	0.69
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.08	0.69
1:D:642:ARG:HD2	1:D:646:HIS:CE1	2.28	0.69
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: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:A:558:ASN:O	1:A:562:LEU:HD22	1.93	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:281:SER:O	1:A:283:THR:HG23	1.94	0.67
1:D:31:VAL:HG12	1:D:32:GLU:N	2.08	0.67
1:B:129:ALA:HB1	1:B:225:TYR:CE2	2.29	0.67
1:A:261:GLU:O	1:A:262:ILE:HD12	1.95	0.67
1:D:793:VAL:HG22	1:D:796:PHE:O	1.94	0.67
3:F:108:DT:H2''	3:F:109:DC:C5'	2.24	0.67
1:A:402:ASN:HA	1:A:886:ALA:O	1.93	0.67
1:D:403:ARG:HD2	1:D:887:ALA:O	1.93	0.67
1:C:83:LEU:N	1:C:83:LEU:HD12	2.09	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:434:PHE:HE1	1:D:461:MET:H	1.41	0.67
1:D:109:ARG:CZ	1:D:142:ILE:HD11	2.25	0.67
1:D:340:PHE:HD1	1:D:343:LEU:HD12	1.60	0.66
1:C:152:LEU:HD11	1:C:161:GLU:HG2	1.76	0.66
1:A:855:THR:HG23	1:A:858:ILE:HG12	1.77	0.66
1:D:219:GLU:OE2	1:D:262:ILE:HG23	1.94	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: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:474:GLU:OE2	1:A:477:LYS:HE2	1.95	0.66
1:A:82:ALA:O	1:A:382:GLN:HB2	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:D:124:PRO:HB3	1:D:131:HIS:HD2	1.61	0.66
1:C:166:ILE:HG22	1:C:175:GLY:HA2	1.76	0.66
1:D:212:ILE:HG22	1:D:212:ILE:O	1.96	0.66
1:D:611:THR:HB	1:D:614:GLU:OE1	1.96	0.66
1:D:365:TRP:CE2	1:D:566:LEU:HD23	2.31	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:316:ASN:ND2	1:B:319:ARG:H	1.93	0.65
1:B:229:ARG:NE	1:B:233:ILE:HD11	2.10	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
2:K:16:DG:H2''	2:K:17:DC:C5'	2.21	0.65
1:C:642:ARG:HD2	1:C:646:HIS:NE2	2.11	0.65
1:C:512:GLU:HB3	1:C:513:PRO:HD2	1.78	0.65
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.79	0.65
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.26	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:B:331:VAL:O	1:B:334:ILE:HG23	1.97	0.65
1:D:31:VAL:HG12	1:D:32:GLU:H	1.59	0.65
1:D:305:TYR:OH	1:D:309:ILE:HB	1.95	0.65
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.77	0.65
1:A:172:GLU:CD	1:A:172:GLU:H	1.99	0.65
1:C:534:SER:O	1:C:538:LEU:HG	1.97	0.65
1:A:653:LYS:HD3	1:A:656:ARG:HH22	1.61	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:C:660:GLU:CB	1:C:661:PRO:HD3	2.27	0.65
1:B:52:ILE:HD12	1:B:428:GLU:HG3	1.79	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
1:D:137:THR:H	1:D:324:ASN:ND2	1.95	0.65
1:A:280:PHE:CD1	1:A:343:LEU:HD23	2.31	0.65
3:L:110:DA:H1'	3:L:111:DT:H5''	1.76	0.65
1:B:495:ASN:OD1	1:B:521:ASP:HA	1.97	0.65
1:C:486:LYS:HD3	1:C:556:GLN:NE2	2.12	0.65
3:J:104:DG:H2''	3:J:105:DC:C5'	2.27	0.65
1:C:818:ASN:HD22	1:C:821:ALA:H	1.45	0.65
2:G:16:DG:H2''	2:G:17:DC:H5''	1.79	0.64
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
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
1:D:283:THR:CG2	1:D:285:GLN:HE22	2.09	0.64
2:E:14:DC:H2''	2:E:15:DC:O5'	1.97	0.64
1:D:825:VAL:HG12	1:D:826:GLU:N	2.12	0.64
1:D:740:ALA:O	1:D:743:LYS:HG2	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:131:HIS:HB2	1:D:225:TYR:OH	1.97	0.64
1:D:594:LEU:O	1:D:598:GLU:HG3	1.98	0.64
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.79	0.64
1:B:412:LEU:HD13	1:B:415:LEU:HD13	1.80	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:489:MET:SD	1:A:553:MET:HG2	2.37	0.64
1:A:314:GLU:CG	1:A:315:SER:N	2.61	0.64
1:D:625:ILE:HG12	1:D:683:MET:HE2	1.80	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:B:164:ILE:HG22	1:B:183:ILE:HD11	1.79	0.64
1:D:191:PHE:HZ	1:D:200:GLU:HB3	1.61	0.64
1:B:167:ALA:HB1	1:B:178:VAL:HG23	1.80	0.64
1:D:812:ASN:HA	1:D:815:ILE:CG1	2.27	0.64
1:A:269:SER:OG	1:A:356:GLN:NE2	2.31	0.64
1:C:411:ASP:OD1	1:C:624:SER:HB3	1.98	0.64
1:C:482:ARG:NE	1:C:556:GLN:HE21	1.91	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:B:215:GLY:O	1:B:273:TYR:HB2	1.98	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:784:SER:HA	1:D:829:LYS:HA	1.80	0.63
1:D:52:ILE:HD12	1:D:428:GLU:HG3	1.81	0.63
1:B:822:PRO:CG	1:B:855:THR:HB	2.28	0.63
1:B:490:LEU:HA	1:B:493:GLN:HG2	1.81	0.63
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.34	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: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:41:CYS:HB2	1:A:42:PRO:HD2	1.80	0.63
1:D:319:ARG:HG2	1:D:319:ARG:HH11	1.64	0.62
1:D:109:ARG:NH1	1:D:208:LYS:HB3	2.14	0.62
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:471:VAL:HG11	1:D:570:LEU:HD11	1.80	0.62
1:C:461:MET:HE3	1:C:581:ARG:CD	2.25	0.62
1:A:514:LEU:HD13	1:A:526:ILE:HG23	1.81	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:D:17:GLU:HG2	1:D:18:ARG:N	2.12	0.62
2:E:6:DA:H2''	2:E:7:DA:C5'	2.29	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:48:LYS:HD2	1:D:49:TYR:CE2	2.35	0.62
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.80	0.62
1:A:636:VAL:O	1:A:640:LYS:HD2	1.99	0.62
1:D:332:LEU:O	1:D:335:ASP:HB3	1.99	0.62
1:A:757:GLU:O	1:A:761:GLN:HG3	1.98	0.62
1:C:544:ARG:HG2	1:C:547:ARG:NH2	2.15	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:645:ASN:O	1:D:649:ASP:HB2	1.99	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:D:434:PHE:CE2	1:D:450:PRO:HB3	2.35	0.62
1:C:149:PHE:O	1:C:197:LEU:HD11	2.00	0.62
3:L:104:DG:H2''	3:L:105:DC:H5'	1.81	0.62
4:A:982:HOH:O	3:F:114:DA:H5'	2.00	0.62
1:D:90:LEU:CD1	1:D:353:ILE:HG22	2.26	0.62
1:C:117:VAL:HG22	1:C:133:ILE:HA	1.82	0.62
1:B:231:LYS:HG3	1:B:232:ASN:N	2.14	0.62
1:C:179:PRO:HB3	1:C:181:GLU:OE1	1.99	0.62
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.82	0.62
1:D:295:GLU:O	1:D:299:ASN:HA	2.00	0.62
1:D:204:PHE:HE1	1:D:208:LYS:HD2	1.65	0.62
1:D:365:TRP:HA	1:D:368:ILE:HD12	1.81	0.62
1:C:116:GLU:HG2	1:C:324:ASN:OD1	2.00	0.61
1:C:356:GLN:H	1:C:356:GLN:NE2	1.98	0.61
1:B:339:GLN:OE1	1:B:339:GLN:HA	2.00	0.61
1:D:269:SER:OG	1:D:355:ILE:HB	1.99	0.61
1:D:356:GLN:OE1	1:D:356:GLN:N	2.33	0.61
1:D:825:VAL:HG12	1:D:826:GLU:H	1.65	0.61
1:A:795:GLY:O	1:A:813:ARG:HD3	2.00	0.61
1:A:197:LEU:HD23	1:A:197:LEU:C	2.20	0.61
1:A:555:ALA:O	1:A:559:ARG:HG2	1.99	0.61
1:A:494:ARG:HD2	1:A:521:ASP:OD1	1.99	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:D:116:GLU:HB3	1:D:320:TYR:OH	2.00	0.61
1:D:202:LEU:O	1:D:206:GLN:HG2	2.01	0.61
1:C:313:ARG:HH11	1:C:313:ARG:HG3	1.66	0.61
1:D:542:LEU:HD12	1:D:545:ALA:HB3	1.81	0.61
1:B:856:ASP:HA	1:B:859:LYS:CB	2.31	0.61
1:A:365:TRP:CD2	1:A:566:LEU:HD23	2.36	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:D:439:LEU:O	1:D:443:ILE:HG13	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: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:812:ASN:CA	1:D:815:ILE:HG12	2.28	0.60
1:D:732:THR:HG22	1:D:745:LEU:HB3	1.83	0.60
1:D:461:MET:HE2	1:D:581:ARG:HH21	1.65	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: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:D:752:MET:CG	1:D:760:LEU:HD12	2.29	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:C:191:PHE:HD2	1:C:196:GLU:HG3	1.66	0.60
1:A:481:GLN:HE21	1:A:559:ARG:NE	2.00	0.60
2:G:16:DG:C2'	2:G:17:DC:H5"	2.32	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
1:A:85:MET:HE2	1:A:87:ASP:N	2.07	0.60
1:A:97:TYR:O	1:A:352:LYS:NZ	2.34	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
3:J:104:DG:C2'	3:J:105:DC:H5"	2.32	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
1:D:516:VAL:HG21	1:D:522:PHE:CE2	2.37	0.59
1:B:606:ASN:HD22	1:B:612:GLU:CA	2.13	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:D:495:ASN:O	1:D:499:ILE:HG13	2.01	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: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:D:802:PRO:HG2	1:D:805:ILE:HG12	1.83	0.59
1:C:449:ARG:HH21	1:C:675:ASN:HB2	1.68	0.59
1:C:482:ARG:HH21	1:C:556:GLN:NE2	2.01	0.59
1:C:323:TYR:HD1	1:C:326:ILE:HD11	1.68	0.59
1:D:152:LEU:HA	1:D:159:VAL:HG22	1.83	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:23:ASN:ND2	1:A:25:ARG:HH12	2.00	0.59
1:B:771:PHE:HD1	1:B:774:LEU:HD12	1.68	0.59
1:A:791:TYR:CD2	1:A:801:CYS:HA	2.37	0.59
2:I:16:DG:H2''	2:I:17:DC:C5'	2.33	0.59
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.68	0.59
1:D:812:ASN:HA	1:D:815:ILE:CD1	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:433:THR:HG22	1:D:461:MET:HE3	1.85	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:C:411:ASP:HB2	1:C:686:GLU:OE2	2.02	0.58
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:D:228:ASN:O	1:D:231:LYS:HG2	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:C:284:ASN:HD21	1:C:829:LYS:NZ	2.00	0.58
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.83	0.58
1:B:305:TYR:HB2	1:B:312:LEU:HD22	1.85	0.58
1:C:878:LYS:HE3	4:I:205:HOH:O	2.03	0.58
1:A:4:PHE:CE1	1:A:20:ILE:HB	2.38	0.58
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.85	0.58
1:A:516:VAL:CG1	1:A:526:ILE:HG21	2.34	0.58
1:B:815:ILE:CD1	1:B:855:THR:HG21	2.28	0.58
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.14	0.58
3:J:104:DG:C1'	3:J:105:DC:H5''	2.33	0.58
1:A:525:GLU:O	1:A:529:LYS:HE3	2.04	0.58
1:A:248:THR:HG22	1:A:265:LEU:HD23	1.85	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:D:402:ASN:ND2	1:D:403:ARG:N	2.50	0.58
1:B:776:TYR:CB	1:B:863:LEU:HD13	2.32	0.58
1:B:297:GLU:O	1:B:298:LEU:HD23	2.04	0.58
1:A:509:SER:O	1:A:534:SER:HB3	2.03	0.58
1:B:494:ARG:O	1:B:498:ILE:HG12	2.04	0.58
1:C:514:LEU:HG	1:C:533:LEU:HD21	1.85	0.58
1:D:469:GLY:C	1:D:472:PRO:HD2	2.24	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:235:GLY:O	1:B:237:SER:N	2.37	0.58
1:B:642:ARG:HB2	1:B:642:ARG:NH1	2.19	0.58
1:D:365:TRP:CD2	1:D:566:LEU:HD23	2.39	0.58
1:A:653:LYS:HD3	1:A:656:ARG:NH2	2.18	0.58
3:J:110:DA:H2''	3:J:111:DT:H5'	1.86	0.58
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:D:160:GLU:HG3	1:D:161:GLU:N	2.19	0.57
1:A:314:GLU:HG3	1:A:315:SER:H	1.68	0.57
1:D:732:THR:HG22	1:D:745:LEU:CB	2.34	0.57
1:C:231:LYS:HG2	1:C:236:GLU:HA	1.85	0.57
1:B:747:GLU:HA	1:B:747:GLU:OE2	2.04	0.57
1:B:133:ILE:HD12	1:B:133:ILE:N	2.18	0.57
1:C:355:ILE:O	1:C:358:VAL:HG13	2.04	0.57
1:C:291:ASP:O	1:C:295:GLU:HG2	2.03	0.57
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.84	0.57
1:A:489:MET:HB3	1:A:552:GLY:HA3	1.86	0.57
1:C:526:ILE:O	1:C:530:ILE:HG13	2.04	0.57
1:B:227:TYR:CD2	1:B:263:ILE:HD13	2.39	0.57
1:D:289:SER:O	1:D:293:ILE:HG12	2.05	0.57
1:C:78:ILE:CG1	1:C:80:LEU:HD23	2.34	0.57
1:A:481:GLN:HE21	1:A:559:ARG:HE	1.52	0.57
1:D:105:HIS:O	1:D:107:LYS:N	2.37	0.57
1:A:101:ILE:HG13	1:A:349:TYR:HB3	1.84	0.57
1:D:118:THR:HB	1:D:313:ARG:NE	2.16	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
2:E:15:DC:H2'	2:E:16:DG:C8	2.39	0.57
1:C:227:TYR:HD2	1:C:228:ASN:ND2	2.02	0.57
1:D:395:PHE:HD2	1:D:594:LEU:HD23	1.68	0.57
1:D:147:TYR:CE1	1:D:187:ILE:HD12	2.40	0.57
1:D:728:MET:HG2	3:L:113:DC:H5''	1.87	0.57
1:A:846:ILE:O	1:A:846:ILE:HG23	2.03	0.57
1:B:514:LEU:H	1:B:541:MET:CE	2.12	0.57
1:B:792:ASP:OD2	1:B:809:LEU:HD22	2.05	0.57
1:C:516:VAL:CG1	1:C:526:ILE:HD13	2.34	0.57
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.85	0.57
1:C:170:LEU:HD22	1:C:170:LEU:N	2.19	0.57
1:B:836:ARG:NH2	1:B:864:HIS:O	2.38	0.57
1:D:40:HIS:CE1	1:D:83:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ASP:CB	1:B:447:ALA:HB2	2.33	0.57
1:B:298:LEU:HD13	1:B:333:GLN:HG2	1.86	0.57
1:A:534:SER:O	1:A:538:LEU:HD12	2.05	0.57
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.85	0.57
1:B:188:TYR:OH	1:B:190:PRO:HB3	2.05	0.57
1:D:194:GLU:O	1:D:198:LEU:HD13	2.03	0.57
1:C:249:ARG:HD3	1:C:251:LYS:HZ1	1.70	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:C:486:LYS:HD3	1:C:556:GLN:CD	2.26	0.56
1:D:700:GLY:HA2	1:D:753:LEU:CD2	2.36	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:71:TRP:O	1:C:75:MET:HG2	2.05	0.56
1:A:857:LEU:CD1	1:A:858:ILE:HG23	2.30	0.56
1:D:573:VAL:HG23	1:D:574:TRP:CD1	2.27	0.56
1:B:299:ASN:HD22	1:B:299:ASN:N	2.03	0.56
1:C:227:TYR:HD2	1:C:228:ASN:HD22	1.51	0.56
1:C:202:LEU:O	1:C:206:GLN:HG2	2.05	0.56
1:C:81:GLU:HG3	1:C:384:ARG:NH2	2.19	0.56
1:C:529:LYS:HG2	1:C:529:LYS:O	2.06	0.56
1:D:679:HIS:O	1:D:680:LEU:HD23	2.05	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:44:SER:O	1:D:46:ALA:N	2.38	0.56
1:C:461:MET:CE	1:C:581:ARG:HB3	2.36	0.56
1:D:513:PRO:HB3	1:D:541:MET:HB2	1.88	0.56
1:B:771:PHE:HA	1:B:774:LEU:HG	1.87	0.56
1:C:760:LEU:HD13	1:C:891:TYR:HA	1.86	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:C:132:PRO:HB3	1:C:229:ARG:HH21	1.71	0.56
3:F:104:DG:H2''	3:F:105:DC:H5'	1.86	0.56
1:D:527:LYS:O	1:D:530:ILE:HG22	2.06	0.56
1:C:11:ILE:HD12	1:C:16:PHE:CD2	2.41	0.56
1:A:8:VAL:O	1:A:354:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:PHE:HE1	1:C:456:CYS:HB3	1.71	0.56
1:D:461:MET:HE1	1:D:581:ARG:HH21	1.69	0.56
1:D:897:LEU:HD12	1:D:898:PHE:N	2.21	0.56
1:D:525:GLU:O	1:D:529:LYS:HG3	2.05	0.56
1:C:193:ASN:ND2	1:C:195:LYS:HB2	2.20	0.56
1:D:761:GLN:NE2	1:D:893:LYS:HA	2.20	0.56
1:A:277:TYR:CE2	1:A:293:ILE:HD12	2.41	0.56
1:D:534:SER:O	1:D:538:LEU:HG	2.06	0.55
1:D:274:ILE:O	1:D:278:LYS:HG3	2.05	0.55
1:B:162:TRP:HZ3	1:B:188:TYR:HB2	1.70	0.55
1:B:123:PHE:CD2	1:B:124:PRO:HD2	2.40	0.55
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.88	0.55
3:L:103:DG:H2''	3:L:104:DG:C8	2.41	0.55
3:F:111:DT:C2'	3:F:112:DT:H5''	2.35	0.55
1:D:243:SER:C	1:D:245:HIS:H	2.09	0.55
3:F:104:DG:C1'	3:F:105:DC:H5''	2.33	0.55
1:A:202:LEU:O	1:A:206:GLN:HG2	2.06	0.55
1:B:121:ASP:OD1	1:B:122:GLY:N	2.32	0.55
1:D:1:MET:HE3	1:D:102:LYS:HE3	1.87	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:A:687:ALA:HB2	1:A:715:MET:CE	2.35	0.55
1:D:760:LEU:HD23	1:D:760:LEU:C	2.27	0.55
1:C:728:MET:CE	3:J:113:DC:H3'	2.36	0.55
1:C:477:LYS:O	1:C:481:GLN:HG3	2.06	0.55
1:D:61:LEU:HD13	1:D:62:PHE:N	2.21	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:B:220:SER:O	1:B:224:PRO:HG2	2.06	0.55
1:D:678:GLN:O	1:D:680:LEU:HG	2.06	0.55
1:D:664:ASP:O	1:D:668:ARG:HG3	2.06	0.55
1:A:731:GLU:H	1:A:731:GLU:CD	2.09	0.55
1:B:316:ASN:HD21	1:B:319:ARG:H	1.53	0.55
1:A:649:ASP:O	1:A:653:LYS:HG2	2.07	0.55
1:C:426:SER:OG	1:C:427:PRO:HD2	2.06	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:A:170:LEU:HD12	1:A:173:GLN:HE21	1.72	0.55
1:B:542:LEU:O	1:B:546:GLN:HG3	2.07	0.55
1:D:145:ARG:NH2	1:D:185:LYS:HG2	2.22	0.55
1:B:494:ARG:HD2	1:B:521:ASP:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:ILE:O	1:C:533:LEU:HB2	2.06	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:487:GLY:HA3	4:B:947:HOH:O	2.05	0.55
1:B:466:ASP:OD2	1:B:467:ARG:N	2.39	0.55
1:B:408:MET:CE	1:B:655:ALA:HB2	2.37	0.55
1:D:449:ARG:HH21	1:D:675:ASN:CB	2.16	0.55
1:C:81:GLU:HG3	1:C:384:ARG:HH22	1.71	0.55
1:B:398:GLU:OE1	1:B:705:LYS:HE3	2.05	0.55
1:D:118:THR:CB	1:D:313:ARG:HE	2.18	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:541:MET:O	1:D:544:ARG:HB2	2.07	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:D:276:LEU:O	1:D:280:PHE:HD1	1.89	0.54
1:B:554:THR:C	1:B:557:ILE:HG22	2.28	0.54
3:F:111:DT:H1'	3:F:112:DT:H5''	1.89	0.54
1:B:397:LYS:HB3	1:B:620:GLY:H	1.71	0.54
3:F:104:DG:H2''	3:F:105:DC:C5'	2.37	0.54
1:D:6:LEU:HB2	1:D:18:ARG:O	2.08	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:160:GLU:H	1:D:317:HIS:CD2	2.24	0.54
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.88	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: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:B:516:VAL:HG11	1:B:526:ILE:HD11	1.89	0.54
1:A:365:TRP:CE2	1:A:566:LEU:HD23	2.42	0.54
1:C:526:ILE:HG22	1:C:530:ILE:HD11	1.89	0.54
1:A:848:TRP:CE2	1:A:854:ILE:HG12	2.42	0.54
1:B:835:LEU:HD21	1:B:846:ILE:HG22	1.89	0.54
1:A:279:LYS:HG3	1:A:280:PHE:CE2	2.43	0.54
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.89	0.54
1:B:373:LEU:HB3	1:B:378:LYS:HB2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH1	1:A:251:LYS:HE2	2.22	0.54
1:B:635:LYS:HG2	1:D:898:PHE:CD2	2.43	0.54
1:C:516:VAL:HG21	1:C:522:PHE:CZ	2.43	0.54
1:A:101:ILE:HD11	1:A:349:TYR:O	2.07	0.54
1:C:365:TRP:CE2	1:C:566:LEU:HD23	2.43	0.54
1:D:87:ASP:OD1	1:D:363:LYS:HE3	2.08	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:122:GLY:HA3	1:D:823:GLN:HE22	1.73	0.54
1:B:416:TYR:O	1:B:420:ILE:HG13	2.08	0.54
1:C:788:ILE:HG13	1:C:826:GLU:OE2	2.07	0.54
1:D:888:LYS:C	1:D:889:LEU:HD12	2.29	0.54
1:C:59:ARG:HH11	1:C:59:ARG:HG2	1.72	0.54
1:C:130:LYS:O	1:C:229:ARG:NH1	2.41	0.54
1:B:635:LYS:HG2	1:D:898:PHE:CE2	2.42	0.54
1:B:809:LEU:O	1:B:813:ARG:HG3	2.08	0.54
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.37	0.54
1:C:214:THR:HG23	1:C:215:GLY:N	2.23	0.54
1:C:301:GLY:O	1:C:330:ARG:NH1	2.41	0.54
1:A:493:GLN:O	1:A:496:GLY:N	2.41	0.54
1:D:450:PRO:HB2	1:D:456:CYS:SG	2.49	0.54
1:D:18:ARG:HA	1:D:27:ARG:O	2.08	0.54
1:A:638:GLU:HB2	4:A:983:HOH:O	2.07	0.54
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: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:B:120:PRO:HA	1:B:310:SER:HB3	1.90	0.53
1:B:163:SER:N	1:B:318:GLN:HE22	2.01	0.53
1:B:115:ILE:HD11	1:B:133:ILE:HG13	1.87	0.53
3:H:105:DC:H2'	3:H:106:DT:H72	1.89	0.53
1:D:204:PHE:CE1	1:D:208:LYS:HD2	2.44	0.53
1:C:318:GLN:HE21	1:C:318:GLN:CA	2.19	0.53
3:J:108:DT:H2''	3:J:109:DC:C5'	2.37	0.53
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.38	0.53
1:A:127:SER:HA	1:A:228:ASN:ND2	2.24	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:771:PHE:HA	1:D:774:LEU:HD12	1.91	0.53
1:D:362:ILE:HG22	1:D:575:PHE:HD1	1.73	0.53
1:D:481:GLN:O	1:D:485:HIS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLU:HB3	1:D:11:ILE:CD1	2.35	0.53
1:A:602:ASN:ND2	1:A:616:PHE:H	2.06	0.53
1:B:824:VAL:CG1	1:B:830:VAL:HG11	2.39	0.53
1:D:61:LEU:HD13	1:D:62:PHE:H	1.73	0.53
1:D:50:PHE:HA	1:D:55:LYS:O	2.08	0.53
1:D:206:GLN:NE2	1:D:241:ARG:HB3	2.20	0.53
1:B:897:LEU:HD23	1:B:897:LEU:N	2.18	0.53
1:D:830:VAL:HG22	1:D:831:TYR:N	2.24	0.53
1:B:835:LEU:HA	1:B:866:MET:HA	1.91	0.53
1:B:198:LEU:O	1:B:200:GLU:N	2.42	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:764:PHE:O	1:B:768:GLU:HG3	2.08	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:D:295:GLU:HG2	1:D:301:GLY:CA	2.28	0.53
1:C:422:GLN:HG3	1:C:678:GLN:O	2.08	0.53
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.38	0.53
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:A:280:PHE:N	1:A:280:PHE:CD2	2.74	0.52
1:D:516:VAL:HG21	1:D:522:PHE:HZ	1.72	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:B:194:GLU:C	1:B:196:GLU:H	2.12	0.52
1:D:105:HIS:C	1:D:107:LYS:H	2.12	0.52
1:A:301:GLY:O	1:A:330:ARG:NE	2.36	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
3:J:101:DG:H2'	3:J:102:DC:C6	2.44	0.52
1:A:784:SER:HB3	1:A:829:LYS:HD3	1.91	0.52
1:D:605:LEU:HA	1:D:608:VAL:HG22	1.91	0.52
1:A:313:ARG:O	1:A:317:HIS:HB2	2.09	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:C:511:ASP:OD2	1:C:533:LEU:HA	2.10	0.52
1:B:340:PHE:O	1:B:343:LEU:HB3	2.09	0.52
1:D:298:LEU:HB2	1:D:300:VAL:CG1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:HE1	1:B:309:ILE:HD11	1.74	0.52
1:B:1:MET:HE1	1:B:24:GLY:CA	2.40	0.52
1:A:422:GLN:HG3	1:A:678:GLN:O	2.10	0.52
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.91	0.52
1:B:167:ALA:HB1	1:B:178:VAL:CG2	2.39	0.52
1:A:263:ILE:N	1:A:263:ILE:HD12	2.25	0.52
1:D:698:ILE:HG12	1:D:752:MET:O	2.09	0.52
1:B:738:PRO:HB3	1:B:780:ALA:O	2.10	0.52
1:C:474:GLU:OE2	1:C:477:LYS:HD2	2.10	0.52
1:C:313:ARG:NH1	1:C:313:ARG:HG3	2.25	0.52
1:B:805:ILE:HD13	1:B:808:ILE:HD12	1.92	0.52
1:B:324:ASN:C	1:B:324:ASN:HD22	2.13	0.52
1:B:112:ASN:ND2	1:B:332:LEU:HD23	2.25	0.52
1:D:189:MET:HB3	1:D:191:PHE:CE1	2.45	0.52
1:C:382:GLN:HB3	1:C:384:ARG:NH1	2.25	0.52
1:D:399:PRO:HB3	1:D:619:TYR:HD2	1.74	0.52
1:A:731:GLU:HG3	1:A:879:PRO:CB	2.39	0.52
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:D:159:VAL:HB	1:D:317:HIS:CD2	2.45	0.51
1:A:290:LEU:O	1:A:294:SER:CB	2.57	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:A:411:ASP:CG	1:A:686:GLU:HG3	2.31	0.51
1:C:154:SER:C	1:C:156:TYR:H	2.14	0.51
1:B:731:GLU:HG3	1:B:879:PRO:HB3	1.92	0.51
1:D:298:LEU:HD11	1:D:333:GLN:HB3	1.91	0.51
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.40	0.51
1:D:509:SER:H	1:D:534:SER:HB3	1.75	0.51
1:D:402:ASN:HD21	1:D:403:ARG:HG2	1.76	0.51
1:B:162:TRP:CZ3	1:B:188:TYR:HB2	2.45	0.51
1:D:250:VAL:HG12	1:D:263:ILE:HD12	1.93	0.51
1:D:757:GLU:O	1:D:761:GLN:HG3	2.11	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:423:VAL:O	1:D:424:ASN:HB3	2.10	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:189:MET:CE	1:D:200:GLU:HG2	2.41	0.51
1:D:800:LYS:HE3	2:K:13:DG:C4'	2.40	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:180:SER:O	1:D:183:ILE:HG22	2.10	0.51
1:D:189:MET:HB3	1:D:191:PHE:HE1	1.76	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
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.75	0.51
1:A:401:PRO:O	1:A:402:ASN:HB2	2.11	0.51
3:L:110:DA:H2''	3:L:111:DT:C5'	2.40	0.51
1:D:251:LYS:HE2	1:D:264:THR:CG2	2.40	0.51
1:D:38:PHE:HE2	1:D:49:TYR:CG	2.29	0.51
1:A:687:ALA:HB2	1:A:715:MET:HE2	1.91	0.51
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.92	0.51
1:A:776:TYR:CD2	1:A:863:LEU:HD21	2.46	0.51
1:D:488:TYR:CE2	1:D:519:ARG:HD2	2.46	0.51
3:J:104:DG:H2''	3:J:105:DC:H5''	1.92	0.51
1:C:660:GLU:HB3	1:C:661:PRO:HD3	1.92	0.51
1:B:308:PRO:O	1:B:312:LEU:N	2.43	0.51
3:J:111:DT:H2'	3:J:112:DT:H71	1.93	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
1:C:121:ASP:HA	1:C:819:ILE:HG12	1.93	0.51
1:C:323:TYR:CD1	1:C:326:ILE:HD11	2.46	0.51
1:A:636:VAL:O	1:A:636:VAL:HG12	2.10	0.51
1:C:167:ALA:O	1:C:178:VAL:HB	2.11	0.51
1:B:880:LEU:O	1:B:884:THR:HG23	2.09	0.51
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.92	0.51
1:D:859:LYS:CG	1:D:860:ASP:H	2.12	0.51
1:B:513:PRO:HG2	1:B:540:GLU:CG	2.41	0.51
1:A:481:GLN:HB3	1:A:559:ARG:HE	1.75	0.51
1:B:824:VAL:HG13	1:B:830:VAL:CG1	2.40	0.51
1:C:81:GLU:CD	1:C:384:ARG:HH12	2.14	0.51
1:B:126:PRO:O	1:B:228:ASN:ND2	2.44	0.51
1:A:23:ASN:HD22	1:A:25:ARG:NH1	2.08	0.51
2:I:16:DG:H2''	2:I:17:DC:H5'	1.92	0.51
1:A:848:TRP:CD2	1:A:854:ILE:HG12	2.46	0.51
1:B:873:GLU:HA	1:B:877:ILE:HB	1.92	0.51
1:D:777:ILE:HD11	1:D:853:GLU:OE1	2.11	0.51
1:C:2:LYS:HE2	1:C:102:LYS:HB3	1.91	0.51
1:C:645:ASN:HD21	1:C:719:ARG:HH11	1.59	0.51
1:B:771:PHE:HE2	1:B:872:LEU:HB2	1.76	0.51
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.92	0.51
1:B:546:GLN:O	1:B:550:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:GLU:HG3	1:D:879:PRO:HB3	1.93	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:D:305:TYR:CD2	1:D:312:LEU:HD22	2.46	0.50
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:530:ILE:HD11	1:D:541:MET:SD	2.51	0.50
1:B:326:ILE:HG23	1:B:330:ARG:HH21	1.76	0.50
1:C:83:LEU:N	1:C:83:LEU:CD1	2.74	0.50
1:D:248:THR:HA	1:D:266:PHE:HD1	1.76	0.50
1:A:664:ASP:O	1:A:668:ARG:HB2	2.10	0.50
1:A:492:ALA:HB1	1:A:549:GLU:HB2	1.92	0.50
1:D:685:ARG:NH1	1:D:714:ASP:OD2	2.42	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:A:2:LYS:CD	1:A:2:LYS:H	1.93	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:A:602:ASN:HD22	1:A:616:PHE:HB2	1.77	0.50
1:A:553:MET:O	1:A:557:ILE:HG12	2.11	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
1:B:252:VAL:HG12	1:B:253:ILE:HG13	1.93	0.50
2:G:6:DA:H2''	2:G:7:DA:C5'	2.41	0.50
1:C:203:ASN:HD22	1:C:203:ASN:N	2.09	0.50
1:D:360:SER:CB	1:D:363:LYS:HB2	2.41	0.50
1:B:188:TYR:CD2	1:B:190:PRO:HD3	2.46	0.50
1:D:475:ILE:CD1	1:D:563:ILE:HG12	2.42	0.50
1:C:500:LYS:HE3	1:C:542:LEU:HD11	1.94	0.50
1:D:397:LYS:HB3	1:D:620:GLY:H	1.77	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:A:38:PHE:CD2	1:A:59:ARG:HA	2.47	0.50
1:A:788:ILE:HD11	1:A:808:ILE:HG21	1.94	0.50
1:D:308:PRO:CG	1:D:311:LYS:HB2	2.36	0.50
1:D:139:TYR:CG	1:D:140:ASP:N	2.80	0.50
1:B:554:THR:O	1:B:557:ILE:HG22	2.11	0.50
1:D:475:ILE:HD11	1:D:563:ILE:HG12	1.92	0.50
1:D:793:VAL:HG23	1:D:796:PHE:HB2	1.94	0.50
1:C:426:SER:HB3	1:C:428:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:NH1	1:D:59:ARG:HG3	2.26	0.50
2:G:6:DA:H2''	2:G:7:DA:H5'	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:441:ASP:HB3	1:C:447:ALA:HB2	1.94	0.50
1:D:317:HIS:HA	1:D:320:TYR:CB	2.42	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:C:404:TYR:CD1	1:C:618:LEU:HD22	2.47	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: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:A:849:PRO:HG2	4:A:933:HOH:O	2.12	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: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:B:12:GLY:CA	1:B:66:ARG:HH11	2.25	0.49
1:A:85:MET:HE3	1:A:85:MET:HA	1.94	0.49
1:D:300:VAL:O	1:D:300:VAL:HG13	2.12	0.49
1:D:229:ARG:NH1	1:D:233:ILE:HD11	2.26	0.49
1:D:305:TYR:HB2	1:D:312:LEU:HD13	1.94	0.49
1:A:494:ARG:O	1:A:498:ILE:HG12	2.12	0.49
1:D:151:LEU:HD23	1:D:151:LEU:C	2.32	0.49
1:B:167:ALA:HA	1:B:176:ASP:H	1.76	0.49
1:D:13:ASP:OD2	1:D:66:ARG:HB2	2.13	0.49
1:C:642:ARG:HH11	1:C:646:HIS:CD2	2.30	0.49
1:A:508:LEU:N	1:A:508:LEU:HD12	2.28	0.49
1:B:471:VAL:O	1:B:475:ILE:HG22	2.13	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: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: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:C:245:HIS:O	1:C:246:ARG:C	2.51	0.49
1:D:512:GLU:CG	1:D:513:PRO:HD2	2.42	0.49
1:B:755:GLU:HB3	1:B:759:SER:CB	2.43	0.49
1:D:313:ARG:HD3	1:D:320:TYR:CZ	2.47	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:D:783:SER:O	1:D:830:VAL:N	2.44	0.49
1:D:298:LEU:C	1:D:300:VAL:H	2.16	0.49
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:A:40:HIS:HD2	1:A:57:CYS:SG	2.36	0.49
1:C:347:MET:HE3	1:C:562:LEU:HD13	1.95	0.49
1:D:437:ALA:HB3	1:D:442:TYR:CZ	2.47	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:D:453:VAL:HG23	1:D:454:TYR:CE2	2.48	0.49
1:B:114:ASP:HB2	1:B:328:VAL:CG2	2.43	0.49
1:A:170:LEU:HA	1:A:177:GLU:HG2	1.94	0.49
1:D:180:SER:HA	1:D:183:ILE:CG2	2.42	0.49
1:D:444:ASN:HA	1:D:599:ARG:NE	2.27	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: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:A:369:ILE:HG12	1:A:474:GLU:HG2	1.94	0.49
1:C:481:GLN:HE21	1:C:559:ARG:NE	2.07	0.49
1:C:846:ILE:HG13	1:C:847:ALA:N	2.27	0.49
1:B:655:ALA:HA	1:B:659:MET:HB2	1.94	0.49
1:C:579:ASP:O	1:C:582:ASN:N	2.46	0.49
1:C:13:ASP:HB3	1:C:64:ASN:HB2	1.93	0.49
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.48	0.49
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:C:449:ARG:NH2	1:C:675:ASN:HB2	2.27	0.48
1:B:248:THR:HG22	1:B:265:LEU:HA	1.95	0.48
1:B:11:ILE:HD13	1:B:247:LYS:HG3	1.95	0.48
1:B:822:PRO:HB2	1:B:849:PRO:HG2	1.96	0.48
1:D:268:ILE:HG22	1:D:269:SER:N	2.27	0.48
1:C:13:ASP:OD2	1:C:64:ASN:HB2	2.12	0.48
1:A:436:VAL:HG12	1:A:437:ALA:O	2.13	0.48
3:H:110:DA:H1'	3:H:111:DT:H5''	1.95	0.48
1:D:112:ASN:HB3	1:D:214:THR:CG2	2.31	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:D:126:PRO:HA	1:D:225:TYR:HD1	1.77	0.48
1:B:472:PRO:HA	1:B:475:ILE:HG22	1.95	0.48
3:J:113:DC:C2'	3:J:114:DA:H5''	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:TYR:O	1:D:307:GLY:N	2.46	0.48
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:A:454:TYR:HB3	1:A:463:TYR:O	2.13	0.48
1:D:93:LEU:HD12	1:D:352:LYS:O	2.12	0.48
1:C:130:LYS:CG	1:C:131:HIS:H	2.13	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:D:434:PHE:CZ	1:D:460:GLY:HA2	2.48	0.48
1:D:698:ILE:O	1:D:753:LEU:O	2.31	0.48
1:D:512:GLU:HG3	1:D:513:PRO:HD2	1.95	0.48
1:D:31:VAL:CG1	1:D:32:GLU:N	2.75	0.48
1:D:599:ARG:HH11	1:D:599:ARG:HG2	1.78	0.48
1:C:6:LEU:HD13	1:C:211:VAL:HG21	1.95	0.48
1:C:642:ARG:HD2	1:C:646:HIS:CE1	2.48	0.48
3:L:104:DG:H2"	3:L:105:DC:C5'	2.42	0.48
1:D:813:ARG:NH2	1:D:842:GLY:HA3	2.29	0.48
1:B:176:ASP:HA	1:B:319:ARG:HH21	1.78	0.48
1:D:512:GLU:CD	1:D:513:PRO:HD2	2.33	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:C:51:ASP:HB2	4:C:919:HOH:O	2.14	0.48
1:C:170:LEU:HD22	1:C:170:LEU:H	1.79	0.48
1:B:302:LYS:HG2	1:B:303:LEU:H	1.79	0.48
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.49	0.48
1:B:456:CYS:SG	1:B:462:MET:HG2	2.53	0.48
1:A:405:LYS:HG2	1:A:406:TYR:CE2	2.49	0.48
1:D:81:GLU:CD	1:D:83:LEU:HD21	2.34	0.48
1:B:217:ASN:HB2	1:B:274:ILE:CD1	2.40	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
2:E:16:DG:H1'	2:E:17:DC:H5"	1.95	0.48
1:C:3:GLU:HG2	1:C:21:ASP:C	2.34	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: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:776:TYR:N	4:B:916:HOH:O	2.46	0.48
1:A:170:LEU:CG	1:A:173:GLN:HE21	2.26	0.48
1:A:152:LEU:HB2	1:A:191:PHE:O	2.14	0.48
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.49	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
1:C:137:THR:OG1	1:C:324:ASN:ND2	2.47	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:C:455:SER:HA	1:C:675:ASN:O	2.13	0.47
1:B:439:LEU:O	1:B:443:ILE:HG13	2.14	0.47
1:C:508:LEU:HD23	1:C:508:LEU:C	2.35	0.47
1:D:752:MET:HE1	1:D:884:THR:HA	1.96	0.47
1:B:775:ASN:O	1:B:779:ILE:HG12	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: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: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:D:687:ALA:HB2	1:D:715:MET:HE1	1.95	0.47
1:B:191:PHE:CD2	1:B:197:LEU:HA	2.49	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: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:A:206:GLN:NE2	1:A:246:ARG:HH22	2.11	0.47
1:D:276:LEU:O	1:D:280:PHE:CD1	2.66	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:B:197:LEU:HD22	1:B:198:LEU:HD23	1.97	0.47
3:H:104:DG:H1'	3:H:105:DC:H5''	1.95	0.47
1:D:514:LEU:N	1:D:541:MET:HE2	2.28	0.47
1:A:598:GLU:HG3	1:A:617:VAL:HG11	1.95	0.47
1:D:411:ASP:HA	1:D:623:ASP:O	2.14	0.47
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.25	0.47
1:D:516:VAL:CG1	1:D:526:ILE:HG21	2.30	0.47
1:D:205:TRP:CD1	1:D:242:LEU:HA	2.49	0.47
1:D:40:HIS:HE1	1:D:83:LEU:HD11	1.80	0.47
1:B:499:ILE:HA	1:B:530:ILE:HD11	1.95	0.47
1:D:7:THR:O	1:D:17:GLU:HA	2.13	0.47
1:D:138:HIS:HD2	1:D:204:PHE:CE2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:ASN:HD22	1:C:821:ALA:N	2.11	0.47
2:E:16:DG:H2''	2:E:17:DC:H5'	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:111:ALA:HB2	1:C:210:PRO:HB3	1.96	0.47
1:D:244:PRO:HG2	1:D:267:GLY:HA3	1.97	0.47
1:B:222:ALA:O	1:B:226:VAL:HG23	2.15	0.47
1:B:136:ILE:HD11	1:B:201:TYR:CE1	2.50	0.47
2:G:17:DC:H2''	2:G:18:DG:O5'	2.15	0.47
1:D:194:GLU:C	1:D:196:GLU:H	2.18	0.47
1:D:591:GLN:HG2	1:D:595:GLN:NE2	2.29	0.47
1:D:28:THR:O	1:D:29:ARG:HB3	2.15	0.47
1:D:527:LYS:C	1:D:530:ILE:HG22	2.34	0.47
1:A:362:ILE:HG22	1:A:363:LYS:N	2.30	0.47
1:D:294:SER:O	1:D:296:PHE:N	2.47	0.47
1:C:818:ASN:HD21	1:C:820:ASP:HB2	1.80	0.47
1:A:481:GLN:NE2	1:A:559:ARG:NE	2.61	0.47
1:C:151:LEU:HD21	1:C:153:ASN:O	2.15	0.47
1:B:804:HIS:CE1	1:B:805:ILE:HG12	2.50	0.47
1:B:524:ASP:C	1:B:526:ILE:H	2.18	0.47
1:C:604:TYR:OH	1:C:658:ARG:HB3	2.15	0.47
3:J:101:DG:H2'	3:J:102:DC:C5	2.50	0.47
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.96	0.47
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.45	0.47
1:B:234:PHE:N	1:B:234:PHE:CD1	2.83	0.47
1:B:292:TYR:C	1:B:292:TYR:CD1	2.88	0.47
1:D:119:SER:OG	1:D:124:PRO:HD3	2.14	0.47
1:C:529:LYS:O	1:C:533:LEU:HD13	2.15	0.47
1:C:17:GLU:HG2	1:C:18:ARG:N	2.28	0.47
1:B:807:GLY:HA2	1:B:845:CYS:O	2.15	0.47
1:B:606:ASN:ND2	1:B:613:GLY:N	2.62	0.47
1:D:162:TRP:HB3	1:D:188:TYR:CZ	2.50	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
1:D:111:ALA:HB1	1:D:139:TYR:O	2.15	0.47
1:A:360:SER:HB3	1:A:363:LYS:HB3	1.97	0.47
1:B:554:THR:HA	1:B:557:ILE:HG21	1.97	0.47
1:D:642:ARG:HG3	1:D:642:ARG:HH11	1.80	0.47
1:C:151:LEU:HD23	1:C:152:LEU:N	2.30	0.47
1:B:159:VAL:HG11	1:B:313:ARG:CG	2.44	0.47
1:D:4:PHE:CE2	1:D:20:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:CD1	1:A:173:GLN:HE21	2.27	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:A:1:MET:HE3	1:A:24:GLY:HA3	1.97	0.47
1:D:506:PRO:O	1:D:508:LEU:HD22	2.14	0.47
1:A:285:GLN:HB3	1:A:292:TYR:HE2	1.79	0.47
1:C:318:GLN:NE2	1:C:318:GLN:CA	2.78	0.47
1:A:279:LYS:CG	1:A:280:PHE:CE2	2.97	0.47
1:C:151:LEU:CD2	1:C:153:ASN:H	2.28	0.47
1:D:286:PRO:O	1:D:829:LYS:HD2	2.14	0.47
1:C:213:LEU:HD13	1:C:223:ILE:HD11	1.96	0.47
1:C:13:ASP:OD2	1:C:66:ARG:HB3	2.15	0.47
1:A:414:SER:O	1:A:417:PRO:HD2	2.15	0.47
1:A:148:VAL:HG21	1:A:325:ILE:HD11	1.97	0.47
1:A:182:ILE:HG21	1:A:329:TYR:CE1	2.49	0.47
1:A:403:ARG:HD2	1:A:887:ALA:O	2.15	0.47
1:A:154:SER:C	1:A:156:TYR:N	2.68	0.47
1:D:516:VAL:HG12	1:D:526:ILE:HD13	1.97	0.46
1:C:503:LEU:HG	1:C:538:LEU:HB3	1.97	0.46
1:C:59:ARG:NH1	1:C:59:ARG:HG2	2.30	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:578:TYR:OH	1:C:580:LEU:HB2	2.15	0.46
1:A:787:ASN:HD22	1:A:790:LYS:HE2	1.78	0.46
1:B:198:LEU:O	1:B:199:MET:C	2.53	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: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:A:671:CYS:SG	1:A:676:ASN:HB2	2.55	0.46
1:A:117:VAL:O	1:A:117:VAL:HG12	2.14	0.46
1:D:543:PHE:CA	1:D:546:GLN:HE21	2.08	0.46
1:D:206:GLN:HE22	1:D:241:ARG:CB	2.22	0.46
1:B:229:ARG:HE	1:B:233:ILE:HD11	1.78	0.46
3:H:107:DG:H2''	3:H:108:DT:OP2	2.14	0.46
1:D:345:LEU:HA	1:D:355:ILE:HD12	1.97	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
3:L:108:DT:H1'	3:L:109:DC:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:HA	1:B:530:ILE:CD1	2.46	0.46
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
1:D:197:LEU:HD23	1:D:197:LEU:C	2.35	0.46
1:D:143:ASP:HB3	1:D:147:TYR:OH	2.15	0.46
1:D:793:VAL:HG23	1:D:793:VAL:O	2.15	0.46
1:B:150:ASP:OD2	1:B:151:LEU:N	2.49	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:68:ALA:O	1:D:72:ILE:HG13	2.16	0.46
1:A:214:THR:HG21	1:A:341:ILE:HD11	1.97	0.46
1:B:489:MET:SD	1:B:553:MET:HG2	2.55	0.46
1:B:458:PRO:HG3	1:B:592:MET:SD	2.56	0.46
1:B:364:THR:HG21	1:B:562:LEU:HD11	1.97	0.46
1:B:862:VAL:O	1:B:862:VAL:HG22	2.15	0.46
1:C:461:MET:HE2	1:C:581:ARG:HB3	1.96	0.46
1:B:133:ILE:HD12	1:B:133:ILE:H	1.81	0.46
1:D:747:GLU:O	1:D:751:ARG:HG3	2.15	0.46
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.96	0.46
1:D:347:MET:SD	1:D:562:LEU:HD11	2.56	0.46
1:B:804:HIS:NE2	1:B:805:ILE:HG12	2.30	0.46
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.50	0.46
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.97	0.46
1:D:556:GLN:O	1:D:556:GLN:NE2	2.48	0.46
1:D:159:VAL:HB	1:D:317:HIS:CG	2.51	0.46
1:B:528:GLU:C	1:B:530:ILE:H	2.19	0.46
1:A:470:VAL:O	1:A:474:GLU:HB2	2.15	0.46
1:A:261:GLU:C	1:A:262:ILE:HD12	2.34	0.46
1:A:653:LYS:O	1:A:657:GLU:HG2	2.16	0.46
1:D:799:PRO:O	1:D:800:LYS:HB2	2.16	0.46
1:A:6:LEU:HD11	1:A:20:ILE:CD1	2.46	0.46
1:A:426:SER:HB3	1:A:429:THR:HG23	1.98	0.46
1:A:492:ALA:CB	1:A:549:GLU:HB2	2.45	0.46
1:D:641:PHE:CG	1:D:647:TRP:HB3	2.51	0.46
1:D:833:LEU:HD22	1:D:866:MET:HE3	1.97	0.46
2:G:12:DA:H61	3:H:106:DT:H3	1.64	0.46
1:C:818:ASN:ND2	1:C:821:ALA:H	2.11	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:A:482:ARG:CZ	1:A:556:GLN:HE21	2.28	0.46
1:D:776:TYR:CD2	1:D:863:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:CD1	1:B:133:ILE:HG12	2.43	0.46
1:D:652:ASP:OD2	1:D:656:ARG:NH1	2.49	0.46
2:G:16:DG:H1'	2:G:17:DC:H5''	1.98	0.46
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:A:516:VAL:HG13	1:A:526:ILE:HG21	1.98	0.46
1:D:630:ASP:O	1:D:632:ILE:N	2.49	0.46
1:C:170:LEU:HD12	1:C:177:GLU:OE2	2.16	0.46
1:B:248:THR:HG22	1:B:265:LEU:HD23	1.97	0.46
1:A:50:PHE:HD2	1:A:54:GLY:O	1.99	0.46
2:I:4:CTG:H2''	2:I:5:DG:OP2	2.16	0.46
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.46	0.45
1:B:834:PRO:O	1:B:866:MET:HA	2.16	0.45
1:A:808:ILE:HD13	1:A:824:VAL:HG11	1.98	0.45
1:C:482:ARG:HH21	1:C:556:GLN:HE22	1.63	0.45
1:D:316:ASN:ND2	1:D:319:ARG:CB	2.78	0.45
1:D:137:THR:HG22	1:D:328:VAL:HG21	1.98	0.45
1:B:808:ILE:HG23	1:B:824:VAL:HG21	1.98	0.45
2:I:16:DG:H2''	2:I:17:DC:H5''	1.98	0.45
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.97	0.45
1:A:833:LEU:HD22	1:A:866:MET:HE3	1.98	0.45
1:B:815:ILE:HG23	1:B:821:ALA:HB3	1.98	0.45
3:H:104:DG:H5''	4:H:161:HOH:O	2.15	0.45
1:D:831:TYR:CD2	1:D:848:TRP:NE1	2.74	0.45
1:D:344:SER:O	1:D:345:LEU:C	2.54	0.45
1:A:420:ILE:HG12	1:A:586:ILE:HD11	1.99	0.45
1:D:351:ALA:HB3	1:D:353:ILE:HG12	1.98	0.45
1:B:200:GLU:O	1:B:204:PHE:N	2.46	0.45
1:A:788:ILE:CD1	1:A:808:ILE:HG21	2.46	0.45
3:H:104:DG:H2''	3:H:105:DC:H5'	1.96	0.45
1:D:344:SER:O	1:D:347:MET:N	2.49	0.45
1:C:426:SER:CB	1:C:428:GLU:OE2	2.65	0.45
1:D:38:PHE:CZ	1:D:59:ARG:HG2	2.51	0.45
1:D:813:ARG:HH22	1:D:843:ASP:H	1.64	0.45
1:D:687:ALA:HB2	1:D:715:MET:CE	2.46	0.45
1:C:647:TRP:CE3	1:C:651:LEU:HD12	2.51	0.45
1:D:789:ALA:O	1:D:792:ASP:HB3	2.17	0.45
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.51	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
1:C:526:ILE:HG22	1:C:530:ILE:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PHE:N	1:D:62:PHE:CD1	2.84	0.45
3:H:111:DT:H2''	3:H:112:DT:OP2	2.17	0.45
1:D:736:SER:HA	1:D:782:VAL:O	2.16	0.45
1:B:391:TYR:HB2	1:B:392:PRO:HD2	1.99	0.45
1:C:451:SER:OG	1:C:452:ASP:N	2.49	0.45
1:C:286:PRO:HD2	1:C:292:TYR:CE1	2.51	0.45
3:L:108:DT:C1'	3:L:109:DC:H5''	2.46	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:D:822:PRO:HB2	1:D:849:PRO:HG2	1.98	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:B:658:ARG:O	1:B:661:PRO:HD2	2.17	0.45
1:D:148:VAL:HG21	1:D:325:ILE:CD1	2.47	0.45
1:B:408:MET:SD	1:B:655:ALA:HB2	2.56	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.99	0.45
1:A:371:ASN:O	1:A:375:GLU:HG2	2.16	0.45
1:D:396:VAL:HG12	1:D:705:LYS:HD3	1.98	0.45
1:D:880:LEU:O	1:D:884:THR:HG23	2.17	0.45
1:D:240:LYS:C	1:D:242:LEU:H	2.20	0.45
1:C:249:ARG:CD	1:C:251:LYS:HZ3	2.28	0.45
1:D:793:VAL:CG2	1:D:796:PHE:HB2	2.47	0.45
1:A:728:MET:HE2	3:F:113:DC:H3'	1.99	0.45
1:C:844:LYS:HZ1	2:I:12:DA:P	2.40	0.45
1:C:116:GLU:HB3	1:C:320:TYR:OH	2.16	0.45
1:D:151:LEU:HD11	1:D:154:SER:OG	2.17	0.45
1:B:333:GLN:O	1:B:336:ALA:HB3	2.15	0.45
3:J:105:DC:H2'	3:J:106:DT:H72	1.98	0.45
1:D:251:LYS:HE2	1:D:264:THR:HG21	1.97	0.45
1:C:233:ILE:HG22	1:C:234:PHE:N	2.31	0.45
1:A:491:ALA:C	1:A:493:GLN:H	2.20	0.45
1:D:395:PHE:CZ	1:D:397:LYS:HB2	2.52	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:D:365:TRP:O	1:D:369:ILE:HG13	2.17	0.45
1:D:285:GLN:HB3	1:D:292:TYR:CE2	2.52	0.45
1:D:800:LYS:H	2:K:13:DG:H5''	1.82	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:D:367:ALA:O	1:D:370:PHE:HB3	2.16	0.45
1:C:685:ARG:HD2	1:C:685:ARG:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.65	0.45
1:C:234:PHE:HB3	1:C:238:THR:HG21	1.99	0.45
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
2:K:15:DC:C2'	2:K:16:DG:C8	2.90	0.45
1:B:606:ASN:ND2	1:B:612:GLU:CA	2.78	0.45
2:K:9:DG:H2''	2:K:10:DA:OP2	2.15	0.45
2:G:12:DA:C2	3:H:107:DG:C2	3.05	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
1:D:114:ASP:HB3	1:D:328:VAL:HG12	1.98	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: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: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:A:214:THR:OG1	1:A:215:GLY:N	2.50	0.45
1:D:484:GLU:C	1:D:486:LYS:N	2.70	0.45
1:D:856:ASP:HA	1:D:859:LYS:HD2	1.99	0.44
1:D:402:ASN:HD22	1:D:403:ARG:N	2.13	0.44
1:D:17:GLU:HG2	1:D:18:ARG:H	1.82	0.44
1:C:52:ILE:HG12	4:C:919:HOH:O	2.16	0.44
2:K:13:DG:H2''	2:K:14:DC:OP2	2.17	0.44
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.85	0.44
1:B:898:PHE:C	1:B:900:MET:H	2.21	0.44
1:A:840:PRO:HD3	1:A:865:TRP:CE2	2.53	0.44
1:B:44:SER:C	1:B:46:ALA:H	2.20	0.44
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.98	0.44
1:B:685:ARG:HD2	1:B:685:ARG:C	2.38	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:503:LEU:HG	1:D:538:LEU:HD13	1.99	0.44
1:C:461:MET:CE	1:C:581:ARG:HD2	2.34	0.44
1:B:502:ALA:HB3	1:B:530:ILE:CG1	2.39	0.44
1:D:514:LEU:HD12	1:D:530:ILE:HB	1.99	0.44
1:B:1:MET:HE3	1:B:20:ILE:CG2	2.47	0.44
1:D:137:THR:N	1:D:324:ASN:ND2	2.63	0.44
1:A:481:GLN:NE2	1:A:559:ARG:HE	2.14	0.44
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:189:MET:O	1:A:191:PHE:CE1	2.71	0.44
1:C:405:LYS:O	1:C:690:GLY:HA2	2.17	0.44
1:B:271:LEU:CD1	1:B:356:GLN:HA	2.46	0.44
1:A:299:ASN:O	1:A:300:VAL:HG13	2.17	0.44
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.88	0.44
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.32	0.44
1:C:520:PHE:O	1:C:521:ASP:C	2.55	0.44
1:B:775:ASN:HB3	1:B:778:SER:OG	2.17	0.44
1:C:426:SER:OG	1:C:428:GLU:OE2	2.34	0.44
1:A:745:LEU:HD13	1:A:876:PHE:HD1	1.82	0.44
1:C:274:ILE:HG23	1:C:275:ASP:N	2.32	0.44
1:D:340:PHE:C	1:D:342:ASN:H	2.19	0.44
1:D:788:ILE:HD11	1:D:825:VAL:O	2.17	0.44
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.33	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:D:497:GLU:O	1:D:498:ILE:HD13	2.18	0.44
1:D:692:PRO:HG3	1:D:713:TRP:HZ2	1.82	0.44
1:C:702:TRP:CZ3	1:C:710:LEU:HD21	2.53	0.44
1:C:12:GLY:C	1:C:14:SER:H	2.20	0.44
1:D:459:ASN:OD1	1:D:584:THR:HG22	2.17	0.44
2:K:11:DC:H2"	2:K:12:DA:C8	2.52	0.44
1:B:800:LYS:HZ1	3:H:108:DT:H5"	1.83	0.44
1:B:608:VAL:HG11	1:D:897:LEU:HD21	2.00	0.44
1:D:294:SER:C	1:D:296:PHE:N	2.70	0.44
1:C:178:VAL:CG2	1:C:322:SER:HB3	2.48	0.44
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.99	0.44
1:C:557:ILE:HD13	1:C:557:ILE:HA	1.84	0.44
1:B:855:THR:HG23	1:B:858:ILE:HG12	2.00	0.44
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.99	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:B:13:ASP:OD1	1:B:66:ARG:HB2	2.18	0.44
3:H:109:DC:H2"	3:H:110:DA:O5'	2.16	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:246:ARG:HH11	1:B:246:ARG:HG3	1.82	0.44
1:B:188:TYR:CE2	1:B:190:PRO:HB3	2.52	0.44
1:D:443:ILE:HD13	1:D:595:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:597:ILE:HD11	1:B:663:ILE:HG23	1.99	0.44
1:D:578:TYR:OH	1:D:580:LEU:HD23	2.18	0.44
1:A:777:ILE:HG23	1:A:831:TYR:CE2	2.53	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:B:729:GLY:O	1:B:734:LYS:HE2	2.17	0.44
1:A:815:ILE:HG22	1:A:857:LEU:HD11	1.99	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:115:ILE:CG1	1:B:116:GLU:H	2.24	0.44
3:H:104:DG:C1'	3:H:105:DC:H5''	2.47	0.44
1:D:830:VAL:CG2	1:D:831:TYR:N	2.81	0.44
1:C:678:GLN:HG2	1:C:680:LEU:HG	1.99	0.44
1:B:506:PRO:CB	1:B:535:ALA:HB2	2.48	0.44
1:D:495:ASN:OD1	1:D:521:ASP:HA	2.18	0.44
1:C:148:VAL:HG11	1:C:325:ILE:HD11	1.99	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:B:658:ARG:C	1:B:661:PRO:HD2	2.39	0.44
1:D:137:THR:CG2	1:D:328:VAL:HG21	2.47	0.44
1:B:425:ILE:HG23	1:B:463:TYR:CE2	2.53	0.44
1:A:546:GLN:O	1:A:547:ARG:C	2.56	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:B:115:ILE:CG1	1:B:116:GLU:N	2.77	0.43
1:A:362:ILE:HD11	1:A:569:ALA:HA	1.99	0.43
3:J:105:DC:H2''	3:J:106:DT:C6	2.53	0.43
1:D:421:ARG:NH1	1:D:479:PHE:CE2	2.84	0.43
1:D:364:THR:HG22	1:D:365:TRP:N	2.33	0.43
1:B:180:SER:O	1:B:183:ILE:HG22	2.19	0.43
1:A:784:SER:HB3	1:A:829:LYS:NZ	2.33	0.43
1:B:434:PHE:HD1	1:B:462:MET:HG3	1.83	0.43
1:A:702:TRP:CD1	1:A:708:TYR:HB3	2.53	0.43
1:C:97:TYR:O	1:C:99:TYR:N	2.47	0.43
1:A:725:LEU:HD22	1:A:753:LEU:HD12	1.99	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:B:582:ASN:O	1:B:586:ILE:HG13	2.18	0.43
1:D:140:ASP:OD1	1:D:141:SER:N	2.51	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:D:248:THR:HG21	1:D:265:LEU:HD23	1.99	0.43
1:A:144:ASP:OD2	1:A:185:LYS:HE2	2.18	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:118:THR:HG21	1:D:313:ARG:HB3	2.00	0.43
1:D:340:PHE:O	1:D:342:ASN:N	2.51	0.43
1:D:143:ASP:C	1:D:145:ARG:N	2.72	0.43
1:D:725:LEU:HD11	1:D:750:ARG:CB	2.48	0.43
1:A:707:ARG:HA	1:A:728:MET:O	2.18	0.43
1:D:437:ALA:HB3	1:D:442:TYR:CE2	2.53	0.43
1:B:301:GLY:O	1:B:302:LYS:HB2	2.18	0.43
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.98	0.43
1:D:23:ASN:HB2	1:D:24:GLY:H	1.57	0.43
1:D:151:LEU:HA	1:D:191:PHE:O	2.19	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: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:D:705:LYS:C	1:D:707:ARG:H	2.21	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:B:191:PHE:CD1	1:B:197:LEU:HG	2.54	0.43
1:D:270:VAL:O	1:D:271:LEU:HG	2.17	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
1:D:305:TYR:C	1:D:307:GLY:H	2.22	0.43
1:A:796:PHE:CE1	1:A:813:ARG:HD2	2.53	0.43
3:J:101:DG:C2'	3:J:102:DC:C6	3.01	0.43
1:A:776:TYR:CG	1:A:863:LEU:HD21	2.53	0.43
1:C:643:ASP:HB2	4:C:1005:HOH:O	2.17	0.43
1:D:859:LYS:O	1:D:863:LEU:HD22	2.19	0.43
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.53	0.43
1:D:550:VAL:CA	1:D:553:MET:HB3	2.45	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:486:LYS:O	1:D:490:LEU:HG	2.19	0.43
1:C:398:GLU:OE1	1:C:705:LYS:HE3	2.18	0.43
1:C:180:SER:O	1:C:182:ILE:N	2.51	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:DG:C2'	2:I:17:DC:H5''	2.48	0.43
1:C:811:TYR:HA	1:C:846:ILE:HD11	2.01	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
1:B:6:LEU:HG	1:B:19:TYR:HA	1.99	0.43
1:D:673:TYR:C	1:D:675:ASN:H	2.20	0.43
1:B:810:THR:CG2	1:B:841:PHE:HB3	2.49	0.43
1:A:426:SER:OG	1:A:427:PRO:HD2	2.18	0.43
1:D:811:TYR:HB2	1:D:846:ILE:HG13	2.01	0.43
1:D:405:LYS:O	1:D:699:GLY:HA3	2.18	0.43
1:D:881:GLU:O	1:D:882:GLY:C	2.57	0.43
1:B:636:VAL:O	1:B:637:GLY:O	2.37	0.43
1:A:518:TYR:H	1:A:518:TYR:HD1	1.62	0.43
1:A:482:ARG:HD2	1:A:556:GLN:HG2	2.01	0.43
1:C:136:ILE:O	1:C:148:VAL:HA	2.19	0.43
1:B:897:LEU:H	1:B:897:LEU:CD2	2.22	0.43
1:B:799:PRO:O	1:B:800:LYS:C	2.57	0.43
1:A:304:LYS:HB2	1:A:304:LYS:HE3	1.69	0.43
1:D:830:VAL:HG22	1:D:831:TYR:O	2.19	0.43
1:B:117:VAL:HB	1:B:124:PRO:HG3	2.01	0.43
1:C:503:LEU:HD21	1:C:538:LEU:HB2	2.00	0.43
2:E:16:DG:C2'	2:E:17:DC:H5''	2.49	0.43
1:D:38:PHE:CE2	1:D:59:ARG:HG2	2.54	0.43
1:B:771:PHE:HD1	1:B:774:LEU:CD1	2.30	0.43
1:A:385:SER:HB2	4:A:959:HOH:O	2.18	0.43
1:D:491:ALA:HA	1:D:521:ASP:OD1	2.19	0.43
1:D:295:GLU:CD	1:D:301:GLY:HA2	2.38	0.43
1:B:178:VAL:O	1:B:179:PRO:C	2.57	0.43
1:D:83:LEU:HD22	1:D:381:PRO:HA	2.00	0.43
1:C:81:GLU:CG	1:C:384:ARG:HH22	2.32	0.43
1:B:159:VAL:HB	1:B:317:HIS:CG	2.54	0.43
2:I:6:DA:H2''	2:I:7:DA:C5'	2.47	0.43
1:A:795:GLY:O	1:A:813:ARG:CD	2.67	0.43
1:D:4:PHE:CZ	1:D:20:ILE:HD13	2.53	0.43
3:H:109:DC:H6	3:H:109:DC:H2'	1.72	0.43
1:A:787:ASN:HB3	1:A:790:LYS:HE2	2.01	0.43
1:D:497:GLU:O	1:D:497:GLU:HG3	2.19	0.43
1:B:45:GLN:O	1:B:47:THR:HG23	2.18	0.43
1:A:121:ASP:N	1:A:121:ASP:OD1	2.52	0.43
1:A:873:GLU:HA	1:A:877:ILE:HB	2.00	0.43
1:C:135:ALA:O	1:C:136:ILE:CG1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLN:NE2	1:D:241:ARG:HD2	2.34	0.42
1:C:540:GLU:O	1:C:544:ARG:HD3	2.18	0.42
1:B:738:PRO:HB2	1:B:778:SER:O	2.19	0.42
1:D:294:SER:OG	1:D:330:ARG:HG2	2.19	0.42
1:B:751:ARG:HA	1:B:755:GLU:HB2	2.01	0.42
1:D:770:GLU:O	1:D:774:LEU:HG	2.18	0.42
1:D:586:ILE:HG22	1:D:587:THR:N	2.34	0.42
1:C:725:LEU:HD11	1:C:750:ARG:HB2	2.01	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
1:D:131:HIS:C	1:D:229:ARG:HE	2.23	0.42
3:L:110:DA:C2'	3:L:111:DT:H5''	2.49	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: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: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: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:B:202:LEU:O	1:B:205:TRP:HB3	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:B:198:LEU:O	1:B:201:TYR:N	2.52	0.42
1:A:808:ILE:O	1:A:811:TYR:HB3	2.18	0.42
1:D:747:GLU:HA	1:D:747:GLU:OE2	2.19	0.42
1:A:347:MET:HE3	1:A:558:ASN:ND2	2.34	0.42
1:B:126:PRO:HB3	1:B:224:PRO:HB2	2.01	0.42
3:L:110:DA:C1'	3:L:111:DT:H5''	2.47	0.42
1:C:51:ASP:OD1	1:C:51:ASP:C	2.57	0.42
1:D:425:ILE:O	1:D:426:SER:HB2	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:542:LEU:O	1:C:546:GLN:HG3	2.19	0.42
1:D:843:ASP:HB3	1:D:844:LYS:H	1.56	0.42
1:B:45:GLN:NE2	1:B:58:THR:OG1	2.53	0.42
1:D:579:ASP:C	1:D:579:ASP:OD2	2.57	0.42
1:C:416:TYR:HB2	1:C:417:PRO:HD3	2.01	0.42
1:B:745:LEU:O	1:B:749:ILE:HG13	2.19	0.42
1:C:362:ILE:CD1	1:C:575:PHE:HB2	2.50	0.42
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:PHE:CZ	1:B:846:ILE:HD12	2.54	0.42
1:B:513:PRO:HB3	1:B:541:MET:HE1	2.01	0.42
1:C:516:VAL:HG12	1:C:526:ILE:HD13	2.01	0.42
1:C:458:PRO:CG	1:C:592:MET:SD	3.07	0.42
1:B:240:LYS:C	1:B:242:LEU:H	2.23	0.42
1:C:85:MET:HA	1:C:380:ILE:HD11	2.02	0.42
1:A:581:ARG:NH1	1:A:581:ARG:HB2	2.34	0.42
1:A:738:PRO:HB3	1:A:780:ALA:O	2.19	0.42
1:D:481:GLN:CB	1:D:559:ARG:NE	2.69	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:D:805:ILE:HD13	1:D:808:ILE:HD12	2.01	0.42
1:B:494:ARG:HG3	1:B:495:ASN:ND2	2.35	0.42
3:H:109:DC:H1'	3:H:110:DA:H5'	2.01	0.42
1:C:180:SER:C	1:C:182:ILE:H	2.22	0.42
1:D:405:LYS:O	1:D:690:GLY:HA2	2.19	0.42
1:A:523:SER:O	1:A:527:LYS:CB	2.68	0.42
1:D:115:ILE:HA	1:D:135:ALA:O	2.20	0.42
1:A:439:LEU:O	1:A:443:ILE:HG13	2.19	0.42
1:D:51:ASP:C	1:D:51:ASP:OD2	2.58	0.42
1:B:846:ILE:O	1:B:846:ILE:HG23	2.19	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:151:LEU:HG	1:D:192:ASP:O	2.18	0.42
1:B:176:ASP:OD2	1:B:318:GLN:HG3	2.19	0.42
1:D:25:ARG:CG	1:D:25:ARG:NH1	2.81	0.42
1:D:761:GLN:HE22	1:D:893:LYS:HA	1.82	0.42
1:C:500:LYS:HE2	1:C:542:LEU:HD21	2.01	0.42
1:A:861:ASP:O	1:A:864:HIS:HB3	2.19	0.42
1:D:873:GLU:HA	1:D:877:ILE:HB	2.02	0.42
1:A:83:LEU:HD12	1:A:83:LEU:N	2.35	0.42
1:B:671:CYS:SG	1:B:676:ASN:HB2	2.59	0.42
2:K:16:DG:H5'	4:K:30:HOH:O	2.20	0.42
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
2:E:6:DA:C1'	2:E:7:DA:H5''	2.45	0.42
1:B:658:ARG:CD	1:D:897:LEU:HD22	2.46	0.42
1:B:228:ASN:O	1:B:231:LYS:HG2	2.20	0.42
1:C:266:PHE:CD1	1:C:266:PHE:N	2.87	0.42
1:C:9:GLU:OE1	1:C:266:PHE:HA	2.19	0.42
1:C:203:ASN:ND2	1:C:203:ASN:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ILE:HD13	1:B:566:LEU:HG	2.01	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:4:PHE:O	1:B:19:TYR:HB2	2.19	0.42
1:B:202:LEU:CD1	1:B:242:LEU:HD13	2.50	0.42
1:A:2:LYS:N	1:A:2:LYS:CD	2.68	0.42
2:E:10:DA:C2'	2:E:11:DC:C5'	2.95	0.42
1:D:391:TYR:HB2	1:D:392:PRO:CD	2.34	0.42
1:D:219:GLU:HB3	1:D:272:ASP:OD2	2.19	0.42
1:D:289:SER:O	1:D:290:LEU:C	2.57	0.42
1:B:315:SER:OG	1:B:316:ASN:N	2.52	0.42
1:A:559:ARG:HA	1:A:562:LEU:HD23	2.01	0.42
1:D:743:LYS:HB2	1:D:743:LYS:HE3	1.90	0.42
1:D:247:LYS:O	1:D:266:PHE:HB2	2.20	0.42
1:C:125:GLU:CD	1:C:126:PRO:HD2	2.40	0.42
1:B:732:THR:HG22	1:B:745:LEU:HB3	2.02	0.42
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.55	0.42
1:A:408:MET:HE1	1:A:655:ALA:HB2	2.01	0.42
1:B:48:LYS:O	1:B:377:ASN:HB3	2.20	0.42
1:A:395:PHE:HB2	1:A:591:GLN:CG	2.34	0.42
1:D:597:ILE:HA	1:D:597:ILE:HD12	1.82	0.42
1:D:7:THR:HG22	1:D:18:ARG:CB	2.48	0.42
1:B:3:GLU:HG3	1:B:20:ILE:O	2.20	0.42
1:D:614:GLU:HG2	1:D:631:LYS:HE3	2.02	0.42
3:L:110:DA:H2''	3:L:111:DT:H5'	2.02	0.42
1:D:285:GLN:C	1:D:287:SER:N	2.72	0.42
3:F:113:DC:H2''	3:F:114:DA:OP2	2.18	0.42
1:B:308:PRO:C	1:B:310:SER:N	2.73	0.42
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.55	0.42
1:B:235:GLY:O	1:B:236:GLU:C	2.58	0.42
1:D:20:ILE:HD12	1:D:107:LYS:CB	2.50	0.42
1:B:365:TRP:CD2	1:B:566:LEU:HD23	2.55	0.42
1:D:599:ARG:HG2	1:D:599:ARG:NH1	2.34	0.42
1:C:572:ASN:O	1:C:578:TYR:HB2	2.20	0.42
1:B:709:ALA:HA	1:B:726:LYS:O	2.20	0.42
1:B:118:THR:HG23	1:B:118:THR:O	2.19	0.42
1:D:495:ASN:HD21	1:D:521:ASP:HA	1.85	0.42
1:D:508:LEU:H	1:D:508:LEU:CD2	2.28	0.42
1:C:728:MET:HE2	3:J:113:DC:H3'	2.02	0.42
1:D:323:TYR:CE1	1:D:326:ILE:HD12	2.54	0.42
2:E:16:DG:H2''	2:E:17:DC:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:HG2	1:C:21:ASP:CA	2.46	0.42
1:C:178:VAL:O	1:C:179:PRO:O	2.38	0.42
1:D:708:TYR:CE1	1:D:728:MET:HB3	2.55	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:D:484:GLU:O	1:D:486:LYS:N	2.53	0.42
1:D:376:GLN:O	1:D:377:ASN:HB2	2.18	0.42
1:D:351:ALA:O	1:D:352:LYS:HB2	2.19	0.41
3:F:103:DG:C2'	3:F:104:DG:H5'	2.49	0.41
1:D:319:ARG:HG2	1:D:319:ARG:NH1	2.33	0.41
1:D:7:THR:CG2	1:D:18:ARG:HE	2.32	0.41
1:C:303:LEU:HD21	1:C:319:ARG:CG	2.49	0.41
1:C:199:MET:HG2	1:C:234:PHE:CE2	2.55	0.41
1:D:729:GLY:N	3:L:113:DC:OP1	2.44	0.41
1:D:685:ARG:HD2	1:D:685:ARG:C	2.40	0.41
1:A:709:ALA:HA	1:A:726:LYS:O	2.20	0.41
1:B:662:ALA:HA	1:B:665:ARG:NH2	2.35	0.41
1:B:480:ASN:O	1:B:483:LYS:HB2	2.20	0.41
3:L:106:DT:H2''	3:L:107:DG:OP2	2.20	0.41
1:C:377:ASN:HA	1:C:377:ASN:HD22	1.68	0.41
1:A:529:LYS:O	1:A:533:LEU:HD11	2.20	0.41
1:D:652:ASP:OD2	1:D:652:ASP:C	2.58	0.41
1:D:273:TYR:O	1:D:273:TYR:HD1	2.03	0.41
1:D:17:GLU:CG	1:D:18:ARG:N	2.82	0.41
1:B:737:THR:HG22	1:B:738:PRO:HD2	2.02	0.41
1:B:738:PRO:HB3	1:B:780:ALA:C	2.40	0.41
1:B:231:LYS:HB2	1:B:231:LYS:HE3	1.83	0.41
1:C:660:GLU:CB	1:C:661:PRO:CD	2.97	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:A:507:ASN:C	1:A:508:LEU:HD12	2.40	0.41
1:A:839:ASN:HA	1:A:840:PRO:HD3	1.77	0.41
1:D:217:ASN:N	1:D:272:ASP:OD1	2.53	0.41
1:B:186:ILE:HG22	1:B:187:ILE:H	1.85	0.41
1:D:830:VAL:CG2	1:D:847:ALA:HB1	2.51	0.41
1:D:19:TYR:O	1:D:27:ARG:N	2.53	0.41
1:D:144:ASP:O	1:D:145:ARG:NE	2.53	0.41
1:D:283:THR:HG21	1:D:285:GLN:HE22	1.83	0.41
1:D:800:LYS:H	2:K:13:DG:C5'	2.33	0.41
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.55	0.41
1:B:598:GLU:HG3	1:B:617:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:SER:O	1:C:459:ASN:N	2.53	0.41
1:D:449:ARG:HA	1:D:450:PRO:HD2	1.90	0.41
1:D:191:PHE:HD2	1:D:197:LEU:HA	1.83	0.41
2:E:6:DA:H2"	4:E:19:HOH:O	2.19	0.41
1:C:189:MET:O	1:C:191:PHE:HE1	2.04	0.41
1:D:479:PHE:CD1	1:D:563:ILE:HD13	2.56	0.41
1:D:285:GLN:HB3	1:D:292:TYR:HE2	1.86	0.41
1:C:167:ALA:O	1:C:176:ASP:O	2.38	0.41
1:D:410:PHE:CD2	1:D:685:ARG:HA	2.56	0.41
1:C:162:TRP:CZ3	1:C:164:ILE:HB	2.55	0.41
1:D:579:ASP:O	1:D:582:ASN:HB2	2.21	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:B:395:PHE:HB2	1:B:591:GLN:CG	2.34	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:B:797:PRO:HB3	1:B:809:LEU:HD12	2.01	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:243:SER:O	1:D:245:HIS:N	2.52	0.41
1:B:739:LYS:O	1:B:740:ALA:C	2.59	0.41
1:C:150:ASP:HB2	1:C:188:TYR:HE1	1.86	0.41
1:D:582:ASN:O	1:D:585:ALA:N	2.54	0.41
1:D:110:VAL:HG11	1:D:341:ILE:HG21	2.03	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:A:219:GLU:HG2	1:A:219:GLU:O	2.21	0.41
1:B:363:LYS:HD3	1:B:363:LYS:HA	1.84	0.41
1:D:449:ARG:NH2	1:D:675:ASN:HB2	2.18	0.41
1:B:810:THR:HB	1:B:845:CYS:O	2.20	0.41
1:C:591:GLN:HB2	1:C:591:GLN:HE21	1.66	0.41
1:B:221:PHE:HE2	1:B:225:TYR:HD1	1.67	0.41
1:A:351:ALA:O	1:A:352:LYS:HB2	2.19	0.41
1:B:308:PRO:C	1:B:310:SER:H	2.24	0.41
1:C:546:GLN:C	1:C:548:THR:N	2.74	0.41
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.55	0.41
1:A:154:SER:O	1:A:156:TYR:N	2.53	0.41
1:D:65:MET:HB3	1:D:88:PHE:CE2	2.55	0.41
1:C:413:THR:O	1:C:414:SER:C	2.58	0.41
1:D:98:ASN:O	1:D:99:TYR:HB3	2.20	0.41
1:B:678:GLN:O	1:B:680:LEU:HG	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:C:708:TYR:CZ	1:C:728:MET:HG3	2.56	0.41
1:D:544:ARG:HH11	1:D:544:ARG:HG3	1.85	0.41
1:D:129:ALA:HA	1:D:225:TYR:HE1	1.84	0.41
1:D:421:ARG:HH11	1:D:421:ARG:HG3	1.86	0.41
1:B:343:LEU:HG	1:B:558:ASN:HD21	1.86	0.41
1:D:415:LEU:O	1:D:419:ILE:HG13	2.21	0.41
1:B:302:LYS:HG2	1:B:303:LEU:N	2.36	0.41
1:D:499:ILE:HB	1:D:542:LEU:HD13	2.03	0.41
1:B:198:LEU:HD13	1:B:230:ILE:HG12	2.03	0.41
1:A:395:PHE:CB	1:A:591:GLN:HG3	2.35	0.41
1:D:812:ASN:C	1:D:815:ILE:HG12	2.41	0.41
2:G:13:DG:N2	3:H:105:DC:N3	2.60	0.41
1:C:80:LEU:N	1:C:80:LEU:HD22	2.35	0.41
1:C:178:VAL:O	1:C:179:PRO:C	2.58	0.41
3:F:111:DT:C1'	3:F:112:DT:H5''	2.50	0.41
1:B:194:GLU:C	1:B:196:GLU:N	2.73	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:D:465:LYS:HZ2	1:D:675:ASN:CG	2.24	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:B:198:LEU:C	1:B:200:GLU:N	2.74	0.41
1:D:500:LYS:C	1:D:503:LEU:H	2.25	0.41
1:D:403:ARG:H	1:D:403:ARG:HG2	1.71	0.41
1:D:241:ARG:HA	1:D:241:ARG:HD3	1.95	0.41
1:D:81:GLU:HG2	1:D:83:LEU:CD2	2.51	0.41
1:D:380:ILE:HA	1:D:381:PRO:HD3	1.84	0.41
1:D:830:VAL:HG23	1:D:848:TRP:C	2.41	0.41
1:A:37:LEU:HD11	1:A:72:ILE:HD11	2.03	0.41
1:C:151:LEU:CD2	1:C:152:LEU:N	2.84	0.41
2:I:7:DA:C8	2:I:8:DT:H72	2.56	0.41
1:D:586:ILE:O	1:D:589:PHE:N	2.54	0.41
1:B:365:TRP:CE2	1:B:566:LEU:HD23	2.55	0.41
1:C:274:ILE:CG2	1:C:275:ASP:N	2.83	0.41
1:A:655:ALA:HA	1:A:659:MET:HB2	2.03	0.41
1:D:14:SER:O	1:D:65:MET:HE1	2.21	0.41
1:D:136:ILE:HB	1:D:149:PHE:HB2	2.03	0.41
1:D:633:ILE:O	1:D:633:ILE:CG2	2.68	0.41
1:B:606:ASN:ND2	1:B:613:GLY:H	2.19	0.41
1:D:116:GLU:CB	1:D:320:TYR:OH	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:DC:H2"	2:G:16:DG:H5'	2.01	0.41
1:D:271:LEU:HD22	1:D:276:LEU:CD2	2.45	0.41
1:A:362:ILE:HD12	1:A:569:ALA:CA	2.48	0.41
1:C:317:HIS:O	1:C:318:GLN:C	2.60	0.41
1:D:793:VAL:C	1:D:795:GLY:H	2.24	0.41
1:C:760:LEU:C	1:C:760:LEU:HD22	2.40	0.41
1:D:102:LYS:NZ	1:D:102:LYS:HB2	2.36	0.41
1:B:496:GLY:O	1:B:542:LEU:HD13	2.21	0.41
1:D:362:ILE:HG22	1:D:575:PHE:CD1	2.52	0.41
1:C:2:LYS:HE2	1:C:102:LYS:CB	2.51	0.41
1:A:38:PHE:CE2	1:A:59:ARG:HB2	2.56	0.41
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.56	0.41
1:B:898:PHE:HE2	1:D:653:LYS:HZ2	1.62	0.41
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:D:189:MET:O	1:D:191:PHE:HD1	2.05	0.40
1:D:809:LEU:C	1:D:809:LEU:HD12	2.42	0.40
1:D:825:VAL:CG1	1:D:826:GLU:H	2.32	0.40
1:A:283:THR:O	1:A:284:ASN:C	2.60	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:1:MET:CE	1:B:20:ILE:HG22	2.51	0.40
1:C:176:ASP:C	1:C:178:VAL:H	2.23	0.40
1:B:114:ASP:HB3	1:B:324:ASN:ND2	2.36	0.40
1:B:781:SER:HB2	1:B:832:VAL:HB	2.03	0.40
1:B:690:GLY:O	1:B:711:ASN:HB3	2.21	0.40
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.56	0.40
1:D:698:ILE:HG13	1:D:753:LEU:HD23	2.02	0.40
1:D:118:THR:O	1:D:313:ARG:NH2	2.53	0.40
1:D:198:LEU:CD2	1:D:230:ILE:HG12	2.49	0.40
1:D:223:ILE:CB	1:D:224:PRO:HD3	2.43	0.40
1:D:740:ALA:O	1:D:741:VAL:C	2.59	0.40
1:B:494:ARG:CG	1:B:495:ASN:ND2	2.84	0.40
1:D:183:ILE:HG23	1:D:184:ASP:N	2.36	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:516:VAL:CG1	1:D:526:ILE:HD13	2.52	0.40
1:D:863:LEU:HD22	1:D:863:LEU:H	1.86	0.40
1:D:791:TYR:HB2	1:D:805:ILE:HG21	2.03	0.40
1:C:40:HIS:HE1	1:C:51:ASP:OD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:CD1	1:A:570:LEU:HD22	2.52	0.40
1:C:529:LYS:CG	1:C:529:LYS:O	2.69	0.40
1:A:38:PHE:HE2	1:A:59:ARG:HB2	1.86	0.40
1:A:152:LEU:HD11	1:A:190:PRO:HB2	2.02	0.40
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.77	0.40
1:D:692:PRO:HG3	1:D:713:TRP:CZ2	2.56	0.40
1:C:605:LEU:HD13	1:C:616:PHE:CD2	2.56	0.40
1:D:188:TYR:CG	1:D:189:MET:N	2.90	0.40
1:B:1:MET:HE3	1:B:20:ILE:HG21	2.02	0.40
1:A:636:VAL:O	1:A:636:VAL:CG1	2.69	0.40
1:C:227:TYR:CD2	1:C:228:ASN:ND2	2.88	0.40
1:C:13:ASP:CG	1:C:64:ASN:HB2	2.42	0.40
1:C:218:VAL:HA	1:C:222:ALA:HB3	2.04	0.40
1:B:108:ILE:O	1:B:110:VAL:HG23	2.21	0.40
1:B:609:CYS:C	1:B:611:THR:N	2.74	0.40
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.57	0.40
1:C:423:VAL:HB	1:C:425:ILE:HG13	2.03	0.40
1:A:386:HIS:HB2	1:A:573:VAL:HB	2.04	0.40
1:C:727:ILE:HD13	1:C:749:ILE:CD1	2.51	0.40
1:D:681:MET:CE	1:D:681:MET:HA	2.52	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:B:272:ASP:CG	1:B:274:ILE:HG22	2.42	0.40
1:D:198:LEU:N	1:D:198:LEU:HD12	2.37	0.40
1:A:497:GLU:C	1:A:499:ILE:N	2.72	0.40
1:D:319:ARG:HD3	1:D:323:TYR:CD1	2.56	0.40
1:C:250:VAL:HG23	1:C:261:GLU:OE2	2.21	0.40
1:D:811:TYR:C	1:D:813:ARG:N	2.74	0.40
1:D:535:ALA:O	1:D:539:ASN:ND2	2.54	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: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%)	15	42
1	B	893/906 (99%)	759 (85%)	107 (12%)	27 (3%)	5	17
1	C	886/906 (98%)	769 (87%)	94 (11%)	23 (3%)	7	21
1	D	886/906 (98%)	681 (77%)	162 (18%)	43 (5%)	3	7
All	All	3555/3624 (98%)	3013 (85%)	437 (12%)	105 (3%)	5	17

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%)	35	69
1	B	774/803 (96%)	737 (95%)	37 (5%)	31	64
1	C	780/803 (97%)	740 (95%)	40 (5%)	29	61
1	D	764/803 (95%)	722 (94%)	42 (6%)	27	58
All	All	3103/3212 (97%)	2950 (95%)	153 (5%)	31	63

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	16,23,24	0.77	1 (6%)	17,35,38	0.64	1 (5%)

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	-	0/7/45/46	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C1'-N1	2.01	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	-2.46	114.36	116.82

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.02	29 (3%) 51 40	21, 41, 114, 141	1 (0%)
1	B	897/906 (99%)	0.74	130 (14%) 3 2	26, 63, 157, 177	13 (1%)
1	C	890/906 (98%)	0.08	22 (2%) 61 50	19, 49, 103, 130	2 (0%)
1	D	890/906 (98%)	0.78	124 (13%) 4 2	62, 103, 147, 163	5 (0%)
2	E	14/18 (77%)	0.48	0 100 100	69, 87, 126, 130	0
2	G	13/18 (72%)	1.74	4 (30%) 1 0	59, 143, 168, 169	0
2	I	16/18 (88%)	-0.19	0 100 100	33, 45, 113, 113	0
2	K	12/18 (66%)	0.69	1 (8%) 14 7	41, 116, 144, 150	0
3	F	14/14 (100%)	0.18	0 100 100	87, 103, 120, 132	0
3	H	13/14 (92%)	1.14	2 (15%) 3 2	137, 149, 163, 168	0
3	J	14/14 (100%)	-0.13	0 100 100	35, 61, 89, 93	0
3	L	13/14 (92%)	0.86	0 100 100	119, 128, 134, 138	0
All	All	3680/3752 (98%)	0.40	312 (8%) 13 7	19, 63, 144, 177	21 (0%)

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	507	ASN	11.8
1	B	821	ALA	11.7
1	B	847	ALA	11.4
1	B	862	VAL	10.6
1	B	785	ALA	10.5
1	B	514	LEU	10.4
1	B	820	ASP	9.9
1	B	812	ASN	8.7
1	B	799	PRO	8.6
1	B	846	ILE	8.6
1	B	809	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	510	VAL	8.3
1	B	801	CYS	7.7
1	B	865	TRP	7.3
1	B	508	LEU	7.3
1	B	538	LEU	6.9
1	D	535	ALA	6.9
1	B	866	MET	6.9
1	B	819	ILE	6.6
1	B	786	ASN	6.6
1	B	861	ASP	6.5
1	B	851	GLY	6.4
1	B	798	GLY	6.4
1	B	503	LEU	6.3
2	G	6	DA	6.2
1	D	819	ILE	6.1
1	B	496	GLY	6.1
1	B	850	SER	6.1
1	B	541	MET	6.1
1	D	523	SER	6.0
1	B	535	ALA	6.0
1	B	818	ASN	5.9
1	D	286	PRO	5.8
1	D	170	LEU	5.8
1	B	822	PRO	5.8
1	B	815	ILE	5.8
1	B	863	LEU	5.8
1	B	811	TYR	5.7
1	D	393	GLY	5.6
1	B	857	LEU	5.6
1	B	542	LEU	5.6
1	B	787	ASN	5.6
1	D	850	SER	5.5
1	C	530	ILE	5.5
1	B	505	ASN	5.5
1	B	825	VAL	5.4
1	B	526	ILE	5.3
1	B	844	LYS	5.3
1	A	530	ILE	5.1
1	B	852	THR	5.1
1	D	179	PRO	5.1
1	B	530	ILE	5.1
1	B	816	LYS	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	516	VAL	5.0
1	B	849	PRO	5.0
1	A	502	ALA	5.0
1	D	395	PHE	5.0
1	B	782	VAL	4.9
1	A	508	LEU	4.9
1	B	509	SER	4.9
1	D	174	GLY	4.9
2	G	7	DA	4.8
1	B	803	PHE	4.8
1	B	791	TYR	4.7
1	D	20	ILE	4.7
1	D	145	ARG	4.7
1	D	507	ASN	4.6
1	B	845	CYS	4.6
1	B	827	GLY	4.5
1	B	813	ARG	4.5
1	A	498	ILE	4.4
1	D	394	ALA	4.4
1	B	802	PRO	4.3
1	B	793	VAL	4.3
1	D	180	SER	4.3
1	D	779	ILE	4.3
1	C	500	LYS	4.3
1	D	514	LEU	4.3
1	B	306	ASP	4.2
1	C	498	ILE	4.2
1	D	120	PRO	4.2
1	B	504	HIS	4.2
1	D	178	VAL	4.1
1	B	797	PRO	4.1
1	B	833	LEU	4.0
1	B	783	SER	4.0
1	B	539	ASN	3.9
1	B	511	ASP	3.9
1	B	497	GLU	3.9
1	D	784	SER	3.9
1	D	504	HIS	3.9
1	B	868	TYR	3.8
1	B	834	PRO	3.8
1	D	786	ASN	3.8
1	B	788	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	541	MET	3.8
1	B	498	ILE	3.8
1	D	817	GLY	3.7
1	A	497	GLU	3.7
1	B	848	TRP	3.7
1	D	339	GLN	3.7
1	B	506	PRO	3.7
1	B	545	ALA	3.7
1	D	513	PRO	3.7
1	D	138	HIS	3.7
1	A	499	ILE	3.7
1	B	790	LYS	3.7
1	D	1	MET	3.7
1	D	192	ASP	3.7
1	B	499	ILE	3.7
1	D	548	THR	3.6
1	B	525	GLU	3.6
1	A	542	LEU	3.6
1	D	522	PHE	3.6
1	B	534	SER	3.6
1	D	16	PHE	3.6
1	B	160	GLU	3.6
1	C	495	ASN	3.6
1	B	800	LYS	3.5
1	D	793	VAL	3.5
1	B	855	THR	3.5
1	B	513	PRO	3.5
1	D	266	PHE	3.5
1	B	817	GLY	3.5
1	B	536	LYS	3.5
1	B	523	SER	3.5
1	D	527	LYS	3.4
1	B	502	ALA	3.4
1	B	522	PHE	3.4
1	B	546	GLN	3.4
1	D	538	LEU	3.4
1	B	120	PRO	3.4
1	B	528	GLU	3.4
1	D	790	LYS	3.4
1	B	789	ALA	3.3
1	D	509	SER	3.3
1	D	539	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	787	ASN	3.3
1	C	499	ILE	3.2
3	H	107	DG	3.2
1	D	545	ALA	3.2
1	B	519	ARG	3.2
1	D	147	TYR	3.2
1	A	504	HIS	3.1
1	B	527	LYS	3.1
1	D	265	LEU	3.1
1	A	500	LYS	3.1
1	B	814	ALA	3.1
1	D	849	PRO	3.1
1	D	811	TYR	3.1
1	D	517	ASP	3.1
1	D	782	VAL	3.1
1	D	792	ASP	3.0
1	C	532	LYS	3.0
1	B	175	GLY	3.0
1	B	305	TYR	3.0
1	D	282	PHE	3.0
2	K	7	DA	3.0
1	D	184	ASP	3.0
1	A	505	ASN	3.0
1	B	842	GLY	3.0
1	D	117	VAL	2.9
1	B	828	GLU	2.9
1	D	162	TRP	2.9
1	B	780	ALA	2.9
1	B	781	SER	2.9
1	D	298	LEU	2.9
1	B	307	GLY	2.9
1	D	198	LEU	2.9
1	D	541	MET	2.9
1	D	329	TYR	2.8
1	D	512	GLU	2.8
1	A	518	TYR	2.8
1	D	491	ALA	2.8
1	C	535	ALA	2.8
1	B	130	LYS	2.8
1	D	262	ILE	2.8
1	D	826	GLU	2.8
1	A	522	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	831	TYR	2.8
1	A	528	GLU	2.7
1	D	498	ILE	2.7
1	B	853	GLU	2.7
1	C	508	LEU	2.7
1	C	533	LEU	2.7
1	D	510	VAL	2.7
1	D	809	LEU	2.7
1	A	501	GLU	2.7
1	B	830	VAL	2.7
1	C	541	MET	2.7
1	D	11	ILE	2.7
1	B	512	GLU	2.7
1	D	832	VAL	2.7
1	B	543	PHE	2.7
1	D	281	SER	2.7
1	D	194	GLU	2.7
1	D	768	GLU	2.7
1	A	516	VAL	2.7
1	D	277	TYR	2.6
1	B	805	ILE	2.6
1	D	537	SER	2.6
1	D	783	SER	2.6
1	B	501	GLU	2.6
1	A	507	ASN	2.6
1	B	518	TYR	2.6
1	A	788	ILE	2.6
1	A	506	PRO	2.6
1	D	202	LEU	2.6
1	D	160	GLU	2.6
2	G	10	DA	2.6
1	B	810	THR	2.5
1	A	509	SER	2.5
1	D	789	ALA	2.5
1	B	867	ASP	2.5
1	D	497	GLU	2.5
1	D	767	PHE	2.5
1	D	129	ALA	2.5
1	A	547	ARG	2.5
1	D	787	ASN	2.5
1	D	771	PHE	2.5
1	D	546	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	534	SER	2.4
1	B	126	PRO	2.4
1	B	533	LEU	2.4
1	D	171	GLN	2.4
1	D	542	LEU	2.4
1	D	166	ILE	2.4
1	B	831	TYR	2.4
1	D	488	TYR	2.4
1	D	559	ARG	2.4
1	D	812	ASN	2.4
1	D	175	GLY	2.4
1	B	172	GLU	2.4
1	D	152	LEU	2.4
1	B	171	GLN	2.4
1	B	858	ILE	2.4
1	D	511	ASP	2.4
1	A	533	LEU	2.4
1	D	519	ARG	2.4
1	D	815	ILE	2.4
1	D	338	ARG	2.4
1	A	510	VAL	2.4
1	B	500	LYS	2.3
1	D	804	HIS	2.3
1	C	301	GLY	2.3
1	B	792	ASP	2.3
1	D	518	TYR	2.3
1	D	848	TRP	2.3
1	D	28	THR	2.3
1	D	105	HIS	2.3
1	B	854	ILE	2.3
1	D	557	ILE	2.3
1	D	446	VAL	2.3
1	C	303	LEU	2.3
1	D	493	GLN	2.3
1	D	119	SER	2.3
1	D	153	ASN	2.3
1	D	115	ILE	2.3
1	D	172	GLU	2.3
1	A	786	ASN	2.3
1	D	505	ASN	2.3
1	B	540	GLU	2.3
1	B	856	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	213	LEU	2.3
1	D	290	LEU	2.3
1	D	827	GLY	2.3
1	D	530	ILE	2.2
1	B	777	ILE	2.2
1	D	536	LYS	2.2
1	B	531	LYS	2.2
1	D	203	ASN	2.2
1	B	128	GLN	2.2
1	C	526	ILE	2.2
1	D	182	ILE	2.2
1	D	164	ILE	2.2
1	C	496	GLY	2.2
1	A	503	LEU	2.2
1	B	774	LEU	2.2
1	B	517	ASP	2.2
1	A	809	LEU	2.2
1	C	537	SER	2.2
1	B	123	PHE	2.2
1	D	113	PHE	2.2
1	D	133	ILE	2.2
1	D	245	HIS	2.2
1	A	493	GLN	2.2
1	C	503	LEU	2.2
1	D	132	PRO	2.1
1	B	524	ASP	2.1
1	C	513	PRO	2.1
1	C	514	LEU	2.1
1	B	843	ASP	2.1
1	C	502	ALA	2.1
1	C	504	HIS	2.1
1	B	494	ARG	2.1
1	D	506	PRO	2.1
1	B	393	GLY	2.1
1	D	248	THR	2.1
1	B	495	ASN	2.1
1	B	127	SER	2.1
2	G	8	DT	2.1
1	A	536	LYS	2.1
1	D	93	LEU	2.1
1	B	529	LYS	2.0
1	D	528	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	105	DC	2.0
1	B	122	GLY	2.0
1	D	520	PHE	2.0
1	D	161	GLU	2.0
1	D	391	TYR	2.0
1	C	522	PHE	2.0
1	C	509	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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.