Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:41 PM GMT

PDB ID	:	3RMC
Title	:	Crystal Structure of a replicative DNA polymerase bound to DNA containing Thymine Glycol
Authors	:	Aller, P.; Duclos, S.; Wallace, S.S.; Doublie, S.
Deposited on	:	2011-04-20
Resolution	:	3.00 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

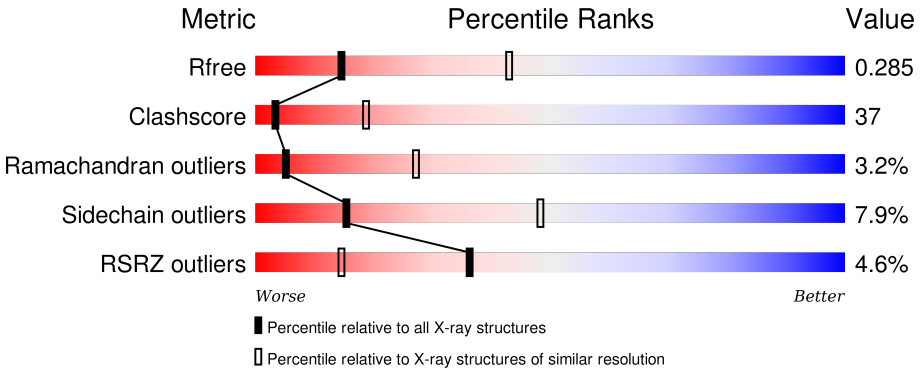
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	3% 45% 47% 7%
1	B	906	8% 47% 47% 5%
1	C	906	% 50% 45% 5%
1	D	906	7% 36% 54% 8%
2	E	18	33% 67%

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Mol	Chain	Length	Quality of chain
2	G	18	11% 89%
2	I	18	39% 50% 11%
2	K	18	6% 44% 33% 22%
3	F	14	7% 86% 7%
3	H	14	21% 79%
3	J	14	50% 50%
3	L	14	7% 7% 86% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31561 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	902	Total	C	N	O	S	0	0	0
			7323	4704	1220	1367	32			
1	B	902	Total	C	N	O	S	13	0	0
			7246	4643	1202	1368	33			
1	C	901	Total	C	N	O	S	0	0	0
			7339	4712	1220	1374	33			
1	D	890	Total	C	N	O	S	15	0	0
			7027	4507	1155	1334	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*TP*(CTG)P*GP*AP*AP*TP*GP *AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			
2	G	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			
2	I	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			
2	K	14	Total	C	N	O	P	0	0	0
			287	136	59	79	13			

- 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	14	Total	C	N	O	P	0	0	0
			282	136	50	83	13			
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	43	Total	O	0	0
			43	43		
4	B	33	Total	O	0	0
			33	33		
4	C	32	Total	O	0	0
			32	32		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	G	3	Total	O	0	0
			3	3		
4	H	3	Total	O	0	0
			3	3		
4	I	3	Total	O	0	0
			3	3		

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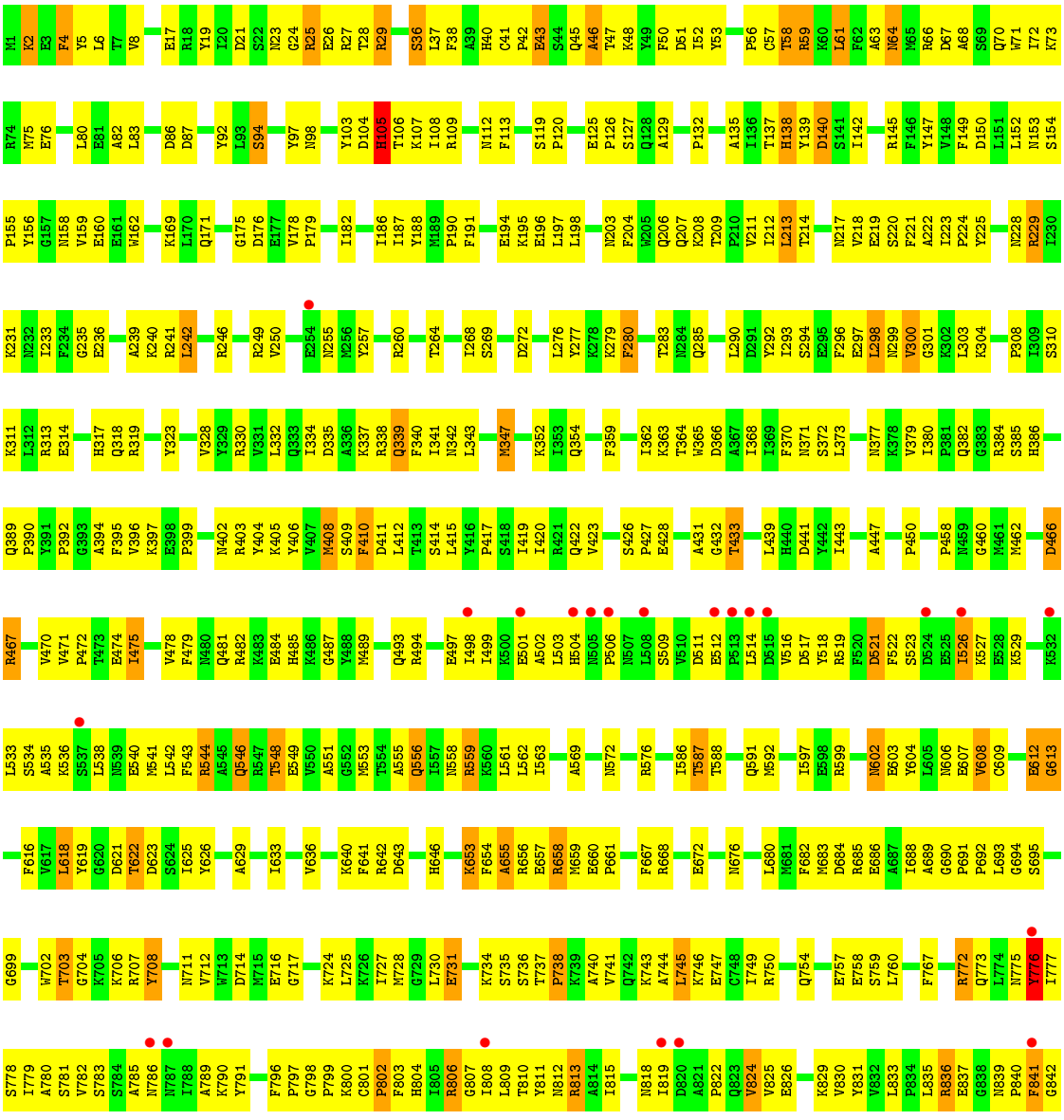
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total O 1 1	0	0

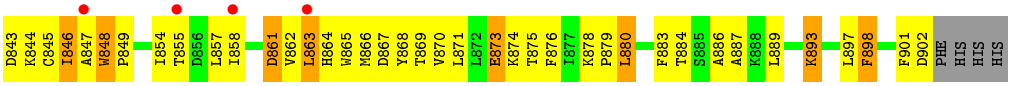
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

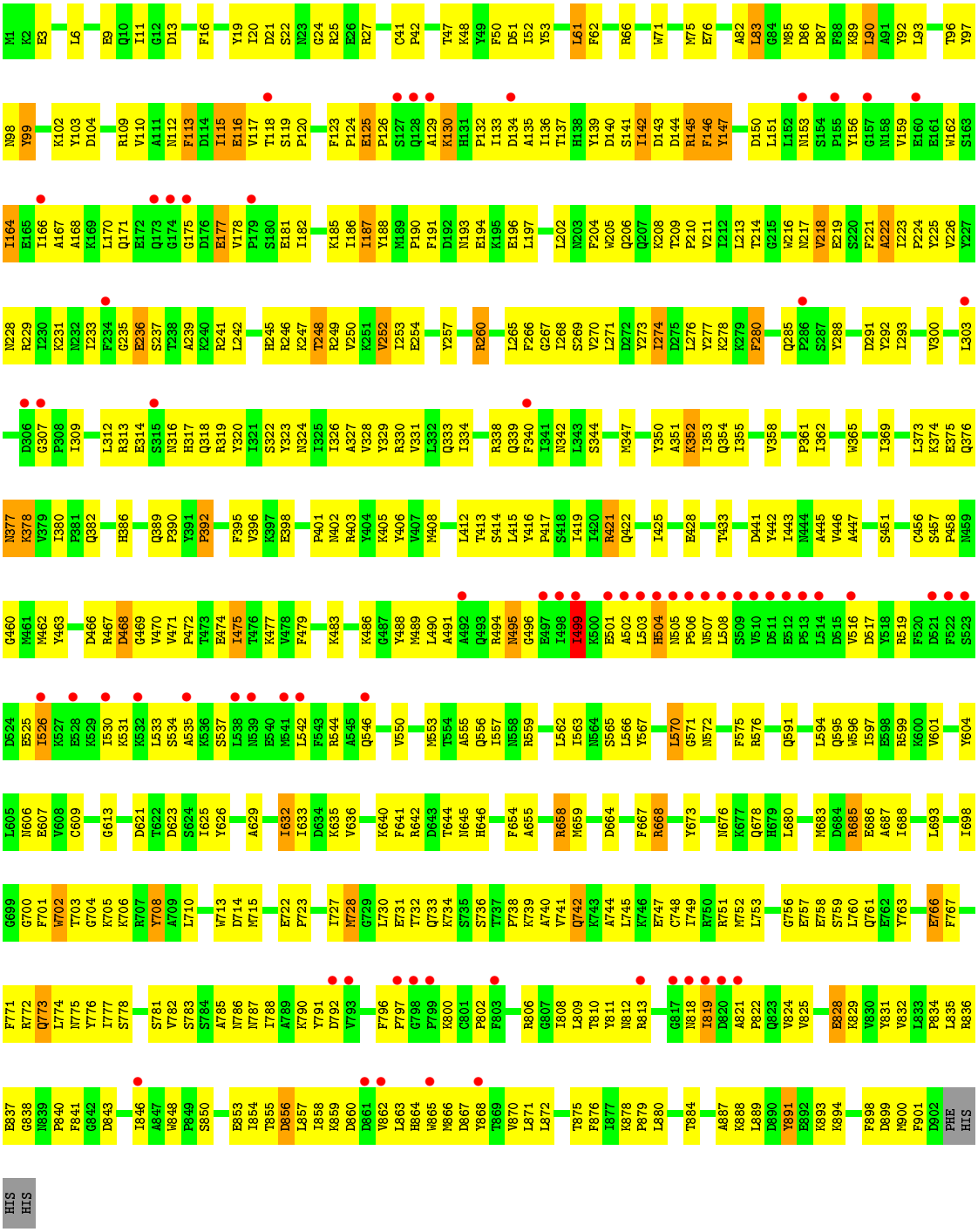
Chain A:





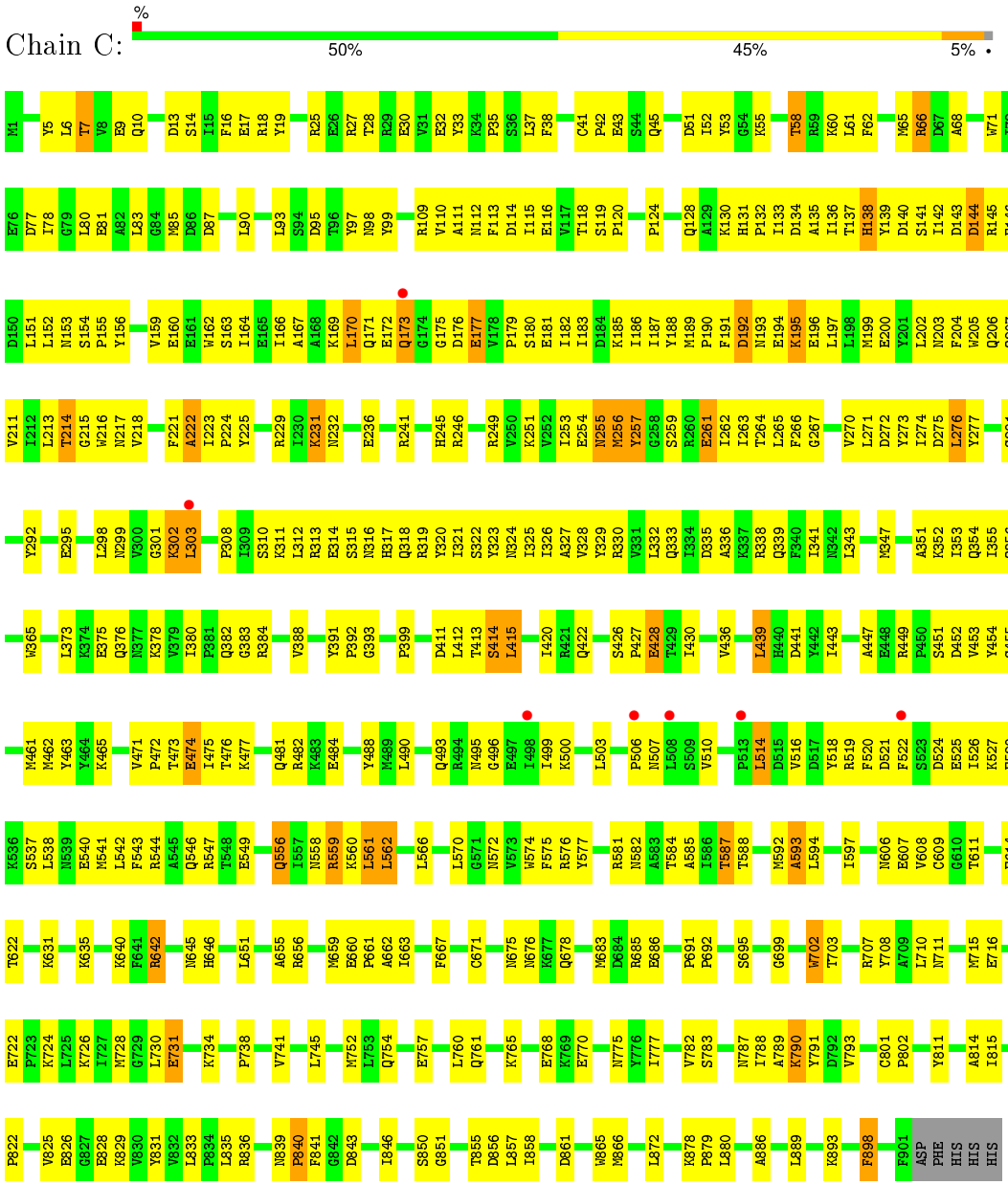
• Molecule 1: DNA polymerase

Chain B:



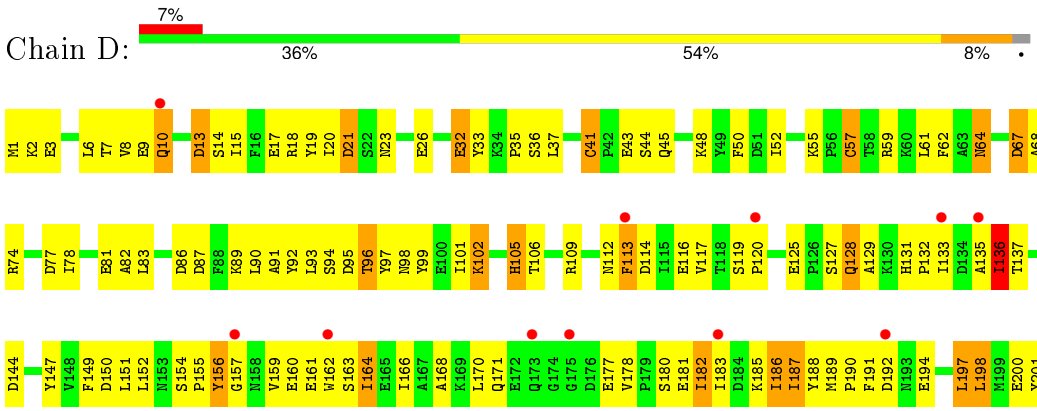
• Molecule 1: DNA polymerase

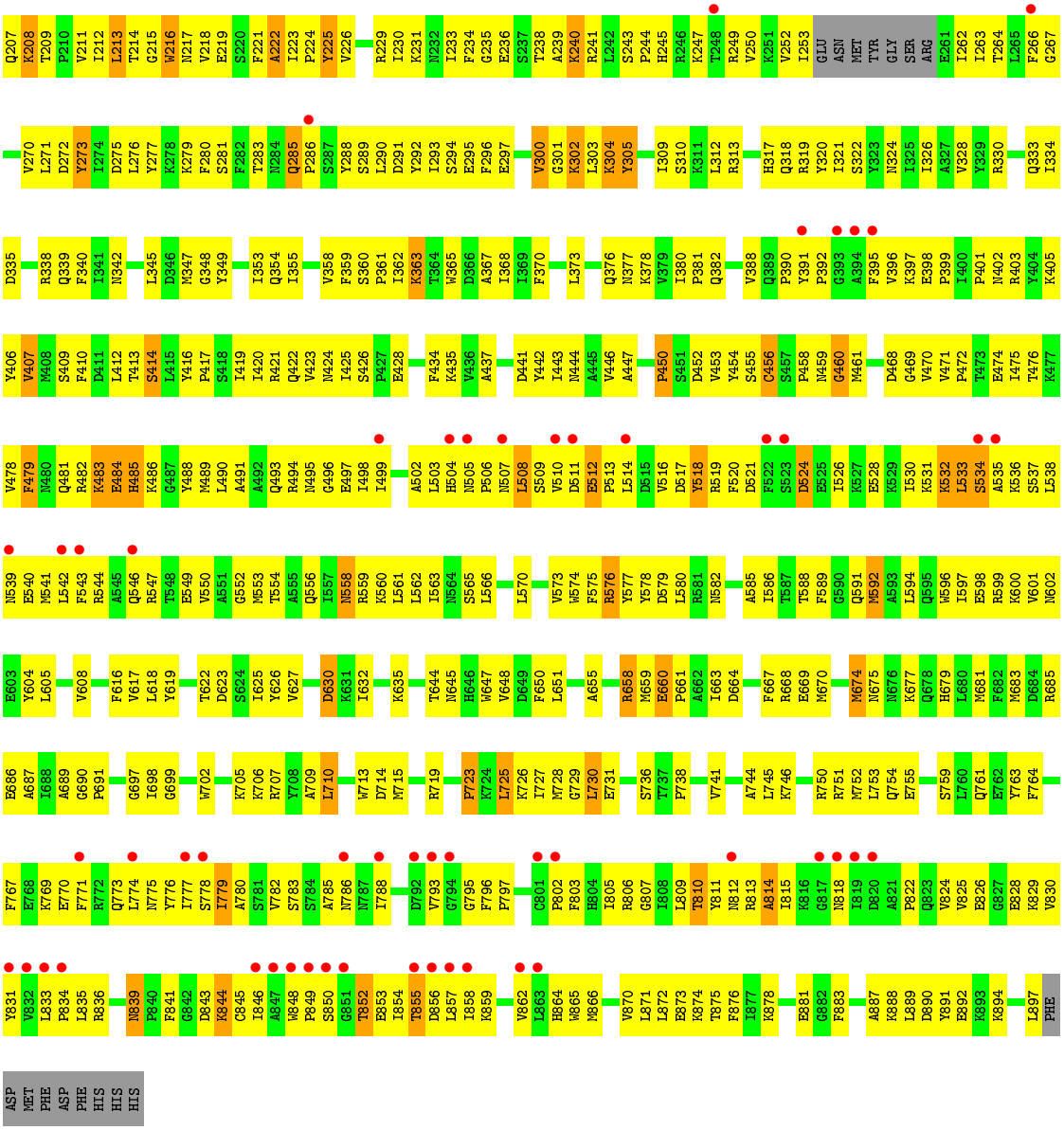
Chain C:



• Molecule 1: DNA polymerase

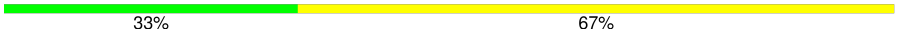
Chain D:

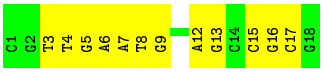




• Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

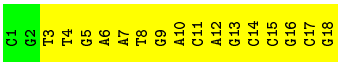
Chain E:





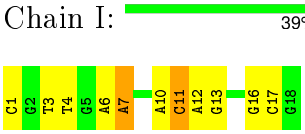
• Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain G:



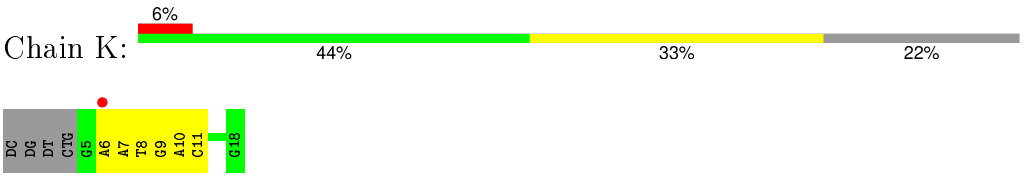
• Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain I:



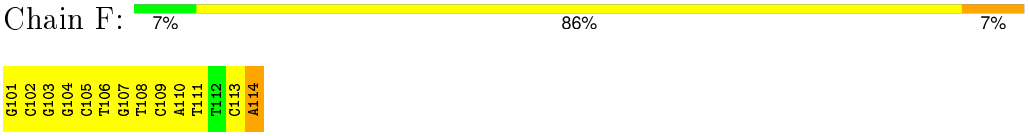
• Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain K:



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

Chain F:



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

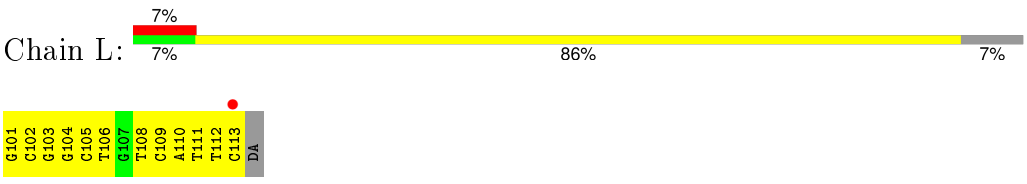
Chain H:

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

Chain J:

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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.99Å 123.77Å 163.64Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-3.00) 96.5 (49.30-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.282 0.223 , 0.285	Depositor DCC
R_{free} test set	10080 reflections (11.29%)	DCC
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 209419 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31561	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	0/7503	0.68	0/10148
1	B	0.42	0/7421	0.62	0/10054
1	C	0.46	0/7519	0.66	0/10166
1	D	0.34	0/7198	0.59	1/9779 (0.0%)
2	E	0.40	0/390	0.71	0/598
2	G	0.39	0/390	0.69	0/598
2	I	0.60	0/390	0.77	0/598
2	K	0.31	0/323	0.67	0/497
3	F	0.33	0/315	0.77	0/484
3	H	0.30	0/315	0.70	0/484
3	J	0.62	0/315	0.89	0/484
3	L	0.28	0/292	0.64	0/449
All	All	0.42	0/32371	0.65	1/44339 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	I	0	2
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	533	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	TYR	Sidechain
3	F	114	DA	Sidechain
2	I	11	DC	Sidechain
2	I	7	DA	Sidechain

5.2 Too-close contacts (i)

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	7323	0	7185	536	0
1	B	7246	0	7027	512	0
1	C	7339	0	7210	456	0
1	D	7027	0	6703	622	0
2	E	370	0	205	19	0
2	G	370	0	205	34	0
2	I	370	0	205	14	0
2	K	287	0	157	11	0
3	F	282	0	158	27	0
3	H	282	0	158	19	0
3	J	282	0	158	21	0
3	L	262	0	149	18	0
4	A	43	0	0	3	0
4	B	33	0	0	2	0
4	C	32	0	0	3	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	1	0
4	I	3	0	0	0	0
4	J	1	0	0	0	0
All	All	31561	0	29520	2248	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 37.

All (2248) 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:D:202:LEU:HD21	1:D:241:ARG:HD3	1.26	1.14
1:D:533:LEU:HD13	1:D:534:SER:H	1.05	1.12
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.32	1.12
1:C:642:ARG:HE	1:C:646:HIS:CD2	1.67	1.12
3:J:104:DG:H2"	3:J:105:DC:H5"	1.20	1.12
2:E:6:DA:H2"	2:E:7:DA:H5'	1.31	1.11
2:E:4:CTG:H5'	2:E:4:CTG:H6	1.33	1.11
1:C:231:LYS:HG2	1:C:236:GLU:HA	1.33	1.10
3:J:104:DG:C2'	3:J:105:DC:H5"	1.85	1.07
3:F:104:DG:H2"	3:F:105:DC:H5"	1.09	1.07
1:B:85:MET:HE2	1:B:87:ASP:H	1.15	1.06
1:B:732:THR:HG23	1:B:733:GLN:HE21	1.20	1.05
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.36	1.04
3:F:104:DG:C2'	3:F:105:DC:H5"	1.87	1.03
1:A:502:ALA:HB1	1:A:538:LEU:HD22	1.42	1.02
1:A:839:ASN:HB2	1:A:840:PRO:HD2	1.42	1.01
1:D:785:ALA:HB1	1:D:788:ILE:HD11	1.41	1.01
1:A:642:ARG:H	1:A:646:HIS:HD2	1.07	1.01
1:D:493:GLN:HG3	1:D:494:ARG:H	1.26	1.00
1:D:815:ILE:HG22	1:D:858:ILE:HG21	1.42	1.00
1:A:362:ILE:HD13	2:E:3:DT:H5'	1.40	1.00
1:D:533:LEU:HD13	1:D:534:SER:N	1.77	0.99
1:A:153:ASN:HD22	1:A:158:ASN:HD22	1.10	0.99
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.26	0.98
1:D:214:THR:HG22	1:D:215:GLY:H	1.26	0.97
1:B:164:ILE:H	1:B:164:ILE:HD13	1.25	0.97
1:C:163:SER:HB3	1:C:318:GLN:HE22	1.29	0.96
1:A:835:LEU:HD11	1:A:846:ILE:HG22	1.43	0.96
1:A:72:ILE:O	1:A:76:GLU:HG3	1.66	0.95
3:L:110:DA:H2"	3:L:111:DT:H5'	1.46	0.94
1:C:195:LYS:NZ	1:C:195:LYS:H	1.64	0.94
1:B:395:PHE:HB2	1:B:591:GLN:HE21	1.32	0.94
2:E:6:DA:H2"	2:E:7:DA:C5'	1.98	0.94
1:B:499:ILE:H	1:B:499:ILE:HD13	1.32	0.94
1:C:711:ASN:HD21	1:C:754:GLN:HE21	0.96	0.94
1:A:703:THR:HG21	1:A:707:ARG:NH1	1.83	0.92
1:D:164:ILE:H	1:D:164:ILE:HD13	1.34	0.92
1:A:836:ARG:NH1	1:A:865:TRP:HA	1.83	0.92
1:B:505:ASN:ND2	1:B:507:ASN:HD22	1.67	0.92
3:F:104:DG:H2"	3:F:105:DC:C5'	1.97	0.92
1:B:217:ASN:H	1:B:274:ILE:HG21	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASN:HD22	1:B:196:GLU:HG2	1.33	0.91
1:C:137:THR:HB	1:C:328:VAL:HG21	1.50	0.91
1:B:83:LEU:HD12	1:B:83:LEU:H	1.35	0.91
1:D:109:ARG:NH1	1:D:142:ILE:HD11	1.85	0.91
1:A:502:ALA:O	1:A:538:LEU:HD13	1.71	0.90
1:C:392:PRO:O	1:C:587:THR:HG21	1.70	0.90
1:A:736:SER:HA	1:A:782:VAL:HB	1.53	0.90
2:K:6:DA:H2"	2:K:7:DA:H5"	1.50	0.90
3:F:110:DA:H2"	3:F:111:DT:H5'	1.54	0.89
1:B:894:LYS:HB2	1:B:894:LYS:NZ	1.87	0.89
1:A:897:LEU:H	1:A:897:LEU:HD12	1.38	0.89
1:B:668:ARG:HG3	1:B:668:ARG:HH11	1.38	0.88
2:E:12:DA:H2"	2:E:13:DG:H5'	1.52	0.88
1:B:219:GLU:HA	1:B:223:ILE:HD12	1.53	0.88
1:D:541:MET:O	1:D:544:ARG:HG2	1.74	0.87
1:A:559:ARG:HH11	1:A:559:ARG:HG2	1.38	0.87
1:D:198:LEU:HD11	1:D:230:ILE:HG12	1.54	0.87
1:D:132:PRO:HA	1:D:229:ARG:HE	1.39	0.87
1:D:481:GLN:HB3	1:D:559:ARG:HE	1.38	0.86
1:A:791:TYR:HB3	1:A:801:CYS:SG	2.15	0.86
1:A:708:TYR:CE2	1:A:728:MET:HG3	2.11	0.86
1:A:25:ARG:HB2	1:A:25:ARG:HH11	1.39	0.86
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.57	0.86
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.74	0.85
1:D:159:VAL:HG12	1:D:160:GLU:H	1.40	0.85
1:B:115:ILE:HG22	1:B:136:ILE:HG23	1.58	0.85
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.42	0.85
1:B:745:LEU:O	1:B:749:ILE:HG13	1.77	0.85
1:C:642:ARG:NH1	1:C:646:HIS:HB3	1.92	0.84
1:D:493:GLN:HG3	1:D:494:ARG:N	1.93	0.84
1:C:855:THR:HG22	1:C:857:LEU:H	1.43	0.84
1:A:127:SER:HA	1:A:228:ASN:ND2	1.92	0.84
1:B:271:LEU:HB3	1:B:276:LEU:HD11	1.59	0.84
2:E:5:DG:H2"	2:E:6:DA:OP2	1.78	0.83
1:D:814:ALA:HB3	1:D:841:PHE:CE1	2.13	0.83
1:D:10:GLN:HA	1:D:15:ILE:HG22	1.59	0.83
2:I:4:CTG:H5"	2:I:4:CTG:H6	1.61	0.83
1:B:777:ILE:HD11	1:B:853:GLU:HG2	1.58	0.83
3:L:104:DG:H2"	3:L:105:DC:C5'	2.09	0.83
2:K:6:DA:H2"	2:K:7:DA:C5'	2.07	0.83
1:A:2:LYS:NZ	1:A:2:LYS:HA	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.42	0.82
1:D:133:ILE:HG12	1:D:229:ARG:HD2	1.62	0.82
1:D:212:ILE:HD11	1:D:345:LEU:HD21	1.62	0.82
1:B:508:LEU:HD23	1:B:508:LEU:H	1.44	0.82
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.59	0.82
1:D:503:LEU:HD11	1:D:539:ASN:HD22	1.42	0.82
1:B:248:THR:HG22	1:B:265:LEU:HA	1.62	0.82
1:A:836:ARG:HH11	1:A:865:TRP:HA	1.44	0.81
1:D:61:LEU:HD23	1:D:62:PHE:N	1.94	0.81
3:L:104:DG:H2"	3:L:105:DC:H5"	1.62	0.81
1:C:836:ARG:HH12	1:C:865:TRP:HA	1.44	0.81
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.61	0.81
1:B:818:ASN:ND2	1:B:821:ALA:HB2	1.95	0.81
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.62	0.81
1:D:164:ILE:HG21	1:D:186:ILE:CD1	2.11	0.81
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.62	0.81
1:A:236:GLU:HG2	1:A:240:LYS:HE2	1.60	0.81
1:C:295:GLU:OE1	1:C:301:GLY:HA2	1.81	0.81
1:A:642:ARG:H	1:A:646:HIS:CD2	1.97	0.80
1:C:818:ASN:ND2	1:C:857:LEU:HD11	1.96	0.80
1:D:803:PHE:HB2	2:K:11:DC:H4'	1.62	0.80
1:D:843:ASP:OD1	1:D:844:LYS:HD3	1.82	0.80
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.63	0.80
1:D:164:ILE:HG21	1:D:186:ILE:HD12	1.63	0.80
1:A:2:LYS:HA	1:A:2:LYS:HZ3	1.46	0.80
1:D:597:ILE:O	1:D:601:VAL:HG23	1.81	0.80
1:D:444:ASN:HA	1:D:599:ARG:NH1	1.96	0.80
1:A:544:ARG:HH11	1:A:544:ARG:HB2	1.45	0.80
1:D:495:ASN:HD22	1:D:521:ASP:HA	1.43	0.80
1:D:140:ASP:HB3	1:D:143:ASP:HB3	1.62	0.80
1:A:303:LEU:HD12	1:A:323:TYR:HA	1.64	0.80
1:B:658:ARG:HG2	1:D:897:LEU:HD21	1.63	0.80
1:D:793:VAL:HG22	1:D:796:PHE:O	1.82	0.80
1:B:808:ILE:HG22	1:B:812:ASN:HD21	1.45	0.80
1:A:422:GLN:NE2	1:A:680:LEU:H	1.79	0.79
1:D:533:LEU:CD1	1:D:534:SER:H	1.93	0.79
1:B:27:ARG:HG3	1:B:27:ARG:HH11	1.47	0.79
1:B:797:PRO:HG3	1:B:806:ARG:NH1	1.97	0.79
1:D:214:THR:HG22	1:D:215:GLY:N	1.96	0.79
1:D:398:GLU:HA	1:D:705:LYS:HE3	1.63	0.79
1:D:109:ARG:HB2	1:D:211:VAL:HG23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:HG12	1:A:572:ASN:ND2	1.97	0.79
1:B:499:ILE:N	1:B:499:ILE:HD13	1.96	0.79
1:D:818:ASN:OD1	1:D:855:THR:HG21	1.82	0.79
1:A:25:ARG:NH1	1:A:25:ARG:HB2	1.98	0.79
1:B:162:TRP:HA	1:B:318:GLN:HE22	1.46	0.79
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.17	0.79
1:C:686:GLU:HG3	1:C:715:MET:CE	2.13	0.79
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.64	0.78
1:B:863:LEU:HD12	1:B:866:MET:HE3	1.66	0.78
1:B:800:LYS:HD3	3:H:108:DT:H4'	1.62	0.78
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.63	0.78
1:C:195:LYS:H	1:C:195:LYS:HZ3	1.31	0.78
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.65	0.78
1:B:534:SER:OG	1:B:537:SER:HB2	1.82	0.78
1:C:73:LYS:NZ	1:C:73:LYS:HB3	1.97	0.78
1:C:642:ARG:HD3	1:C:642:ARG:N	1.99	0.78
1:A:43:GLU:CD	1:A:43:GLU:H	1.87	0.78
3:F:106:DT:H1'	3:F:107:DG:H5'	1.66	0.78
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.65	0.78
1:C:642:ARG:NE	1:C:646:HIS:CD2	2.51	0.77
1:B:505:ASN:HD22	1:B:507:ASN:HD22	1.32	0.77
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.65	0.77
1:D:132:PRO:HA	1:D:229:ARG:NE	1.99	0.77
1:A:127:SER:HA	1:A:228:ASN:HD22	1.48	0.77
3:J:104:DG:H2"	3:J:105:DC:C5'	2.10	0.77
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.48	0.77
1:D:150:ASP:HB3	1:D:188:TYR:HE1	1.48	0.77
1:D:598:GLU:CG	1:D:617:VAL:HG21	2.14	0.77
2:E:4:CTG:H2'	2:E:4:CTG:O6	1.84	0.77
1:D:494:ARG:O	1:D:497:GLU:HG2	1.85	0.77
2:K:6:DA:C2'	2:K:7:DA:H5"	2.15	0.77
1:B:322:SER:O	1:B:326:ILE:HG12	1.85	0.77
1:B:151:LEU:HA	1:B:191:PHE:O	1.84	0.77
1:D:182:ILE:HD13	1:D:182:ILE:O	1.86	0.77
1:B:218:VAL:O	1:B:223:ILE:HG13	1.84	0.76
1:B:751:ARG:HH11	1:B:759:SER:HB3	1.49	0.76
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.67	0.76
1:D:849:PRO:HG2	1:D:852:THR:OG1	1.85	0.76
1:B:222:ALA:O	1:B:226:VAL:HG23	1.83	0.76
2:I:6:DA:H2"	2:I:7:DA:H5'	1.67	0.76
1:C:373:LEU:HB3	1:C:378:LYS:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLN:HE21	1:A:546:GLN:C	1.88	0.76
1:B:818:ASN:HD22	1:B:821:ALA:HB2	1.47	0.76
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.68	0.76
1:A:25:ARG:CB	1:A:25:ARG:HH11	1.99	0.76
1:C:62:PHE:CE2	1:C:68:ALA:HA	2.21	0.76
1:D:305:TYR:OH	1:D:312:LEU:HB2	1.85	0.76
1:D:815:ILE:HG21	1:D:858:ILE:HD13	1.68	0.76
1:C:836:ARG:NH1	1:C:865:TRP:HA	2.01	0.76
3:J:105:DC:H2'	3:J:106:DT:H71	1.68	0.75
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.67	0.75
2:I:4:CTG:C6	2:I:4:CTG:H5"	2.16	0.75
1:C:482:ARG:HH12	1:C:556:GLN:HE21	1.32	0.75
1:D:407:VAL:HG13	1:D:689:ALA:HB3	1.68	0.75
3:L:110:DA:H2"	3:L:111:DT:C5'	2.16	0.75
1:C:85:MET:HA	1:C:380:ILE:HD11	1.69	0.75
1:A:428:GLU:OE2	1:A:428:GLU:N	2.20	0.75
1:A:139:TYR:CE2	1:A:332:LEU:HD21	2.21	0.75
1:A:384:ARG:HD3	1:A:385:SER:N	2.02	0.74
1:C:195:LYS:HZ3	1:C:195:LYS:N	1.84	0.74
1:B:854:ILE:HD11	1:B:858:ILE:HG13	1.68	0.74
1:D:738:PRO:HB3	1:D:780:ALA:O	1.87	0.74
1:B:166:ILE:H	1:B:166:ILE:HD12	1.51	0.74
1:D:512:GLU:CB	1:D:513:PRO:HA	2.17	0.74
1:A:153:ASN:HD22	1:A:158:ASN:ND2	1.83	0.74
1:A:847:ALA:O	1:A:848:TRP:HB3	1.86	0.74
1:C:216:TRP:O	1:C:217:ASN:HB2	1.87	0.74
1:D:856:ASP:HA	1:D:859:LYS:HB2	1.68	0.74
1:D:835:LEU:HD12	1:D:835:LEU:O	1.87	0.74
1:D:202:LEU:CD2	1:D:241:ARG:HD3	2.11	0.74
1:B:775:ASN:HD21	1:B:777:ILE:HB	1.53	0.74
1:A:404:TYR:CD1	1:A:618:LEU:HD13	2.23	0.74
1:D:82:ALA:N	1:D:382:GLN:HE21	1.86	0.74
1:C:231:LYS:HG2	1:C:236:GLU:CA	2.16	0.74
1:D:97:TYR:HB3	1:D:101:ILE:HD11	1.67	0.74
1:A:653:LYS:HD3	1:A:657:GLU:CD	2.07	0.74
1:D:117:VAL:HG13	1:D:132:PRO:O	1.88	0.73
1:A:171:GLN:HE22	1:A:319:ARG:HH12	1.35	0.73
1:A:636:VAL:O	1:A:640:LYS:HD2	1.88	0.73
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.67	0.73
2:E:8:DT:H2'	2:E:9:DG:C8	2.23	0.73
2:K:10:DA:H2"	2:K:11:DC:H5'	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ASN:HD22	1:A:857:LEU:HD11	1.54	0.73
1:D:229:ARG:NH1	1:D:233:ILE:HD11	2.04	0.73
1:D:441:ASP:HB3	1:D:447:ALA:HB2	1.70	0.73
1:C:642:ARG:HD3	1:C:642:ARG:H	1.50	0.73
1:B:193:ASN:ND2	1:B:196:GLU:HG2	2.03	0.73
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.70	0.73
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.70	0.73
1:B:516:VAL:HG13	1:B:544:ARG:HH11	1.52	0.73
1:D:81:GLU:OE2	1:D:83:LEU:HD21	1.89	0.73
1:C:180:SER:O	1:C:183:ILE:HG22	1.88	0.73
1:C:163:SER:HB3	1:C:318:GLN:NE2	2.04	0.73
1:B:83:LEU:N	1:B:83:LEU:HD12	2.03	0.73
1:D:597:ILE:HG12	1:D:683:MET:HE1	1.71	0.73
1:A:392:PRO:O	1:A:587:THR:HG21	1.89	0.73
1:A:501:GLU:HA	1:A:504:HIS:ND1	2.04	0.72
3:H:106:DT:H1'	3:H:107:DG:H5'	1.71	0.72
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.02	0.72
1:A:482:ARG:HH21	1:A:556:GLN:HE22	1.36	0.72
1:D:204:PHE:CE1	1:D:208:LYS:HG3	2.25	0.72
1:D:62:PHE:HB3	1:D:67:ASP:OD1	1.89	0.72
1:C:109:ARG:NH1	1:C:208:LYS:HA	2.03	0.72
1:B:446:VAL:HG22	1:B:446:VAL:O	1.87	0.72
1:D:140:ASP:OD1	1:D:142:ILE:HG12	1.89	0.72
1:A:862:VAL:O	1:A:864:HIS:N	2.23	0.72
1:B:217:ASN:OD1	1:B:274:ILE:HD13	1.90	0.72
1:A:808:ILE:O	1:A:811:TYR:HB3	1.90	0.72
1:D:222:ALA:O	1:D:226:VAL:HG23	1.89	0.72
1:D:398:GLU:CA	1:D:705:LYS:HE3	2.19	0.72
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.70	0.72
1:D:326:ILE:O	1:D:330:ARG:HG2	1.90	0.72
3:J:104:DG:C3'	3:J:105:DC:H5"	2.19	0.71
1:B:749:ILE:HG22	1:B:753:LEU:HD12	1.70	0.71
1:B:621:ASP:OD1	3:H:114:DA:H5'	1.90	0.71
1:D:802:PRO:HD2	1:D:805:ILE:HD12	1.72	0.71
1:A:153:ASN:ND2	1:A:158:ASN:HD22	1.85	0.71
1:D:495:ASN:ND2	1:D:521:ASP:HA	2.05	0.71
1:B:781:SER:HB2	1:B:832:VAL:HB	1.72	0.71
2:G:14:DC:H2"	2:G:15:DC:H5"	1.73	0.71
1:B:347:MET:CE	1:B:562:LEU:HD11	2.21	0.71
1:A:40:HIS:HD2	1:A:57:CYS:SG	2.14	0.71
1:A:818:ASN:ND2	1:A:857:LEU:HD11	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ARG:HA	1:C:660:GLU:HG3	1.73	0.71
1:C:109:ARG:HH12	1:C:208:LYS:CD	2.04	0.71
1:A:706:LYS:HE3	3:F:113:DC:O2	1.91	0.71
1:C:322:SER:O	1:C:326:ILE:HG13	1.90	0.71
1:D:434:PHE:CE1	1:D:460:GLY:HA2	2.26	0.71
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.18	0.71
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.05	0.71
2:I:10:DA:H2"	2:I:11:DC:H5'	1.72	0.71
1:D:846:ILE:HD11	1:D:862:VAL:HG11	1.71	0.70
1:B:517:ASP:OD1	1:B:519:ARG:HB2	1.91	0.70
1:C:176:ASP:OD2	1:C:319:ARG:HD3	1.89	0.70
1:C:272:ASP:OD1	1:C:274:ILE:HG22	1.90	0.70
1:D:535:ALA:HB1	1:D:539:ASN:ND2	2.05	0.70
1:D:322:SER:O	1:D:326:ILE:HG12	1.90	0.70
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.72	0.70
1:D:109:ARG:NH2	1:D:208:LYS:HB3	2.06	0.70
1:D:109:ARG:HH11	1:D:142:ILE:HD11	1.55	0.70
1:C:183:ILE:HD12	1:C:186:ILE:HD12	1.72	0.70
1:B:732:THR:CG2	1:B:733:GLN:HE21	2.02	0.70
1:A:707:ARG:NH2	1:A:731:GLU:OE1	2.25	0.70
1:D:41:CYS:HB3	1:D:57:CYS:HA	1.72	0.70
1:C:711:ASN:HD21	1:C:754:GLN:NE2	1.81	0.70
1:B:811:TYR:OH	1:B:822:PRO:HG2	1.91	0.70
1:B:312:LEU:O	1:B:312:LEU:HD13	1.92	0.70
1:B:408:MET:CE	1:B:685:ARG:HD3	2.22	0.70
1:A:536:LYS:HD3	1:A:536:LYS:O	1.92	0.70
1:C:587:THR:HG22	1:C:588:THR:N	2.05	0.70
1:A:642:ARG:NH1	1:A:642:ARG:HB2	2.07	0.70
1:A:514:LEU:HD12	1:A:526:ILE:HG23	1.73	0.70
1:C:13:ASP:OD2	1:C:66:ARG:HB2	1.91	0.70
1:D:597:ILE:HG21	1:D:683:MET:HE1	1.74	0.69
1:B:785:ALA:HB1	1:B:788:ILE:HD11	1.74	0.69
1:A:362:ILE:CD1	1:A:572:ASN:HD22	2.05	0.69
1:B:164:ILE:HD13	1:B:164:ILE:N	2.05	0.69
1:A:384:ARG:HD3	1:A:385:SER:H	1.56	0.69
1:D:82:ALA:HB3	1:D:382:GLN:HG3	1.75	0.69
1:B:875:THR:O	1:B:879:PRO:HG3	1.92	0.69
1:D:114:ASP:HB3	1:D:328:VAL:HG13	1.73	0.69
2:E:12:DA:H2"	2:E:13:DG:C5'	2.22	0.69
1:B:326:ILE:O	1:B:330:ARG:HG2	1.92	0.69
1:C:176:ASP:O	1:C:177:GLU:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.25	0.69
1:D:330:ARG:O	1:D:334:ILE:HG13	1.92	0.69
1:B:204:PHE:HE1	1:B:208:LYS:HD2	1.57	0.69
1:D:204:PHE:O	1:D:208:LYS:HG2	1.92	0.69
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.75	0.69
1:A:335:ASP:OD2	1:A:341:ILE:HG12	1.92	0.69
1:D:6:LEU:HB2	1:D:18:ARG:O	1.93	0.69
1:C:655:ALA:O	1:C:660:GLU:HG2	1.93	0.69
1:D:149:PHE:HB3	1:D:197:LEU:CD2	2.21	0.69
1:B:732:THR:HG23	1:B:733:GLN:NE2	2.03	0.69
1:A:606:ASN:HD21	1:A:613:GLY:N	1.91	0.69
1:D:234:PHE:HB3	1:D:238:THR:HB	1.74	0.69
2:I:16:DG:H2"	2:I:17:DC:O5'	1.92	0.69
1:C:382:GLN:HG2	1:C:383:GLY:N	2.07	0.69
1:D:201:TYR:O	1:D:204:PHE:HB3	1.92	0.69
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.75	0.69
1:A:474:GLU:O	1:A:478:VAL:HG23	1.92	0.69
1:C:524:ASP:HA	1:C:527:LYS:HE2	1.75	0.68
1:D:811:TYR:HA	1:D:841:PHE:CZ	2.27	0.68
1:D:214:THR:CG2	1:D:215:GLY:H	2.04	0.68
1:C:354:GLN:HB3	1:C:356:GLN:OE1	1.93	0.68
1:A:606:ASN:HD21	1:A:613:GLY:CA	2.05	0.68
1:D:373:LEU:HD12	1:D:380:ILE:HG22	1.75	0.68
1:C:482:ARG:NH1	1:C:560:LYS:HB2	2.08	0.68
1:B:217:ASN:H	1:B:274:ILE:CG2	2.05	0.68
1:D:777:ILE:HG22	1:D:777:ILE:O	1.94	0.68
1:C:14:SER:OG	1:C:30:GLU:HG2	1.92	0.68
1:C:449:ARG:HH12	1:C:452:ASP:HA	1.58	0.68
1:D:147:TYR:HA	1:D:187:ILE:HG23	1.76	0.68
1:D:159:VAL:HG11	1:D:317:HIS:CB	2.24	0.68
1:D:159:VAL:HG11	1:D:317:HIS:HB3	1.76	0.68
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.75	0.68
1:D:132:PRO:CA	1:D:229:ARG:HH21	2.07	0.68
1:C:791:TYR:CE2	1:C:802:PRO:HD3	2.28	0.68
1:A:466:ASP:OD2	1:A:467:ARG:HD3	1.95	0.67
1:A:308:PRO:HG2	1:A:311:LYS:HG2	1.74	0.67
1:D:658:ARG:HH11	1:D:658:ARG:HG3	1.57	0.67
1:A:64:ASN:HD22	1:A:64:ASN:C	1.97	0.67
1:B:894:LYS:HB2	1:B:894:LYS:HZ2	1.57	0.67
1:B:6:LEU:HG	1:B:19:TYR:HA	1.76	0.67
1:D:159:VAL:HG12	1:D:160:GLU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ILE:HD12	1:D:294:SER:N	2.10	0.67
1:D:214:THR:CG2	1:D:273:TYR:HB2	2.24	0.67
1:A:835:LEU:HD21	1:A:846:ILE:CG2	2.25	0.67
1:C:145:ARG:HB2	1:C:147:TYR:HE1	1.60	0.67
1:C:188:TYR:O	1:C:189:MET:HG3	1.94	0.67
1:A:502:ALA:CB	1:A:538:LEU:HD22	2.23	0.67
1:D:797:PRO:HG2	1:D:806:ARG:NH1	2.09	0.67
1:D:775:ASN:HB3	1:D:778:SER:OG	1.95	0.67
1:A:621:ASP:OD2	3:F:114:DA:H5'	1.95	0.67
1:B:641:PHE:HA	1:B:646:HIS:HD2	1.58	0.67
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.77	0.67
1:D:509:SER:HB2	1:D:532:LYS:O	1.95	0.67
1:A:824:VAL:HG13	1:A:849:PRO:HG3	1.76	0.67
1:C:170:LEU:HD23	1:C:177:GLU:HG2	1.77	0.67
1:B:553:MET:O	1:B:557:ILE:HG12	1.94	0.67
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.25	0.67
1:C:28:THR:O	1:C:28:THR:HG23	1.95	0.67
1:A:544:ARG:HB2	1:A:544:ARG:NH1	2.10	0.67
1:C:221:PHE:O	1:C:224:PRO:HD2	1.94	0.67
1:B:134:ASP:OD1	1:B:151:LEU:HB3	1.95	0.67
2:G:16:DG:H2"	2:G:17:DC:H5"	1.77	0.67
1:B:98:ASN:O	1:B:99:TYR:HB3	1.94	0.67
1:B:483:LYS:O	1:B:486:LYS:HG2	1.95	0.67
2:G:4:CTG:H6	2:G:4:CTG:H5"	1.76	0.67
3:F:101:DG:H2"	3:F:102:DC:O5'	1.95	0.67
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.58	0.67
1:B:766:GLU:HG3	1:B:767:PHE:N	2.09	0.67
1:B:319:ARG:HH11	1:B:319:ARG:HG2	1.60	0.66
1:A:347:MET:HB2	1:A:558:ASN:OD1	1.94	0.66
1:B:894:LYS:HB2	1:B:894:LYS:HZ3	1.60	0.66
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.25	0.66
1:D:533:LEU:CD1	1:D:534:SER:N	2.55	0.66
1:B:499:ILE:HG12	1:B:542:LEU:HD13	1.77	0.66
1:D:505:ASN:N	1:D:506:PRO:HD3	2.10	0.66
1:D:561:LEU:HD23	1:D:561:LEU:O	1.96	0.66
1:B:700:GLY:HA2	1:B:753:LEU:HD21	1.76	0.66
1:A:642:ARG:HH11	1:A:642:ARG:HB2	1.60	0.66
1:B:216:TRP:HA	1:B:274:ILE:HG22	1.78	0.66
1:D:481:GLN:CB	1:D:559:ARG:HE	2.08	0.66
1:B:351:ALA:O	1:B:352:LYS:HB2	1.94	0.66
1:A:83:LEU:HD12	1:A:83:LEU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:SER:HB3	1:D:283:THR:HG22	1.78	0.66
1:B:102:LYS:HD2	1:B:103:TYR:H	1.60	0.66
1:B:728:MET:HG3	3:H:113:DC:H5'	1.78	0.66
1:B:599:ARG:HG2	1:B:599:ARG:HH11	1.60	0.66
1:D:504:HIS:C	1:D:506:PRO:HD3	2.14	0.66
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.77	0.66
1:C:193:ASN:HD22	1:C:195:LYS:NZ	1.94	0.66
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.30	0.66
1:D:15:ILE:HD11	1:D:92:TYR:CD2	2.31	0.66
1:B:253:ILE:HD12	1:B:254:GLU:H	1.59	0.66
1:A:730:LEU:HB3	1:A:883:PHE:CZ	2.31	0.66
3:H:110:DA:H2"	3:H:111:DT:C5'	2.26	0.66
1:D:685:ARG:HD2	1:D:685:ARG:C	2.17	0.66
1:B:749:ILE:HG22	1:B:753:LEU:CD1	2.26	0.65
1:B:326:ILE:HG23	1:B:330:ARG:CZ	2.26	0.65
1:A:712:VAL:HG22	1:A:724:LYS:O	1.96	0.65
1:C:757:GLU:HB2	1:C:889:LEU:HD22	1.76	0.65
1:C:439:LEU:HD12	1:C:443:ILE:HD11	1.78	0.65
1:B:186:ILE:HG22	1:B:187:ILE:N	2.11	0.65
1:D:396:VAL:HB	2:K:7:DA:OP1	1.97	0.65
1:C:130:LYS:HE3	1:C:131:HIS:CE1	2.29	0.65
1:A:403:ARG:HD2	1:A:887:ALA:O	1.96	0.65
3:J:110:DA:H2"	3:J:111:DT:C5'	2.27	0.65
1:D:517:ASP:OD1	1:D:519:ARG:HG2	1.96	0.65
1:A:485:HIS:C	1:A:487:GLY:H	1.98	0.65
1:D:151:LEU:HD11	1:D:154:SER:OG	1.97	0.65
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.25	0.65
1:D:112:ASN:HB3	1:D:214:THR:HB	1.77	0.65
3:L:104:DG:H2"	3:L:105:DC:H5'	1.79	0.65
1:D:594:LEU:O	1:D:597:ILE:HG22	1.96	0.65
1:D:216:TRP:CZ2	1:D:293:ILE:HG12	2.32	0.65
1:A:203:ASN:O	1:A:207:GLN:HG2	1.97	0.65
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.31	0.65
1:D:813:ARG:HG3	1:D:814:ALA:H	1.60	0.65
1:C:109:ARG:HH12	1:C:208:LYS:HD3	1.62	0.65
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.26	0.65
1:C:726:LYS:HG3	1:C:728:MET:HE3	1.79	0.65
1:D:149:PHE:CE2	1:D:201:TYR:HA	2.32	0.65
1:A:71:TRP:CZ3	1:A:82:ALA:HB1	2.32	0.65
1:C:818:ASN:HB2	4:C:921:HOH:O	1.97	0.64
1:D:598:GLU:HG2	1:D:617:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:HB2	1:C:384:ARG:HH22	1.60	0.64
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.13	0.64
1:B:777:ILE:CD1	1:B:853:GLU:HG2	2.27	0.64
1:A:396:VAL:HG22	1:A:621:ASP:OD1	1.98	0.64
1:D:604:TYR:O	1:D:608:VAL:HG23	1.97	0.64
1:C:114:ASP:HB3	1:C:328:VAL:HG22	1.77	0.64
2:G:11:DC:H2"	2:G:12:DA:H5'	1.78	0.64
3:F:102:DC:H2"	3:F:103:DG:OP2	1.96	0.64
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.77	0.64
1:D:783:SER:HA	3:L:111:DT:OP1	1.97	0.64
1:B:668:ARG:NH1	1:B:668:ARG:HG3	2.07	0.64
1:C:147:TYR:HB3	1:C:149:PHE:HE1	1.62	0.64
1:D:761:GLN:HG2	1:D:891:TYR:C	2.18	0.64
1:C:153:ASN:HB2	1:C:192:ASP:O	1.98	0.64
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.33	0.64
1:B:501:GLU:HG3	1:B:501:GLU:O	1.96	0.64
1:D:164:ILE:H	1:D:164:ILE:CD1	2.11	0.64
1:D:355:ILE:O	1:D:358:VAL:HG23	1.96	0.64
1:A:540:GLU:O	1:A:544:ARG:HD3	1.98	0.64
1:C:271:LEU:HB3	1:C:276:LEU:CD2	2.28	0.64
1:B:636:VAL:O	1:B:640:LYS:HG3	1.97	0.64
1:A:621:ASP:O	3:F:114:DA:H4'	1.97	0.64
1:D:78:ILE:O	1:D:78:ILE:HG22	1.98	0.64
1:A:470:VAL:O	1:A:474:GLU:HG2	1.98	0.64
1:B:338:ARG:O	1:B:339:GLN:HB2	1.96	0.64
2:G:14:DC:C2'	2:G:15:DC:H5"	2.28	0.64
1:D:163:SER:HB2	1:D:166:ILE:CD1	2.28	0.64
1:C:302:LYS:HE3	1:C:302:LYS:HA	1.78	0.64
1:B:362:ILE:HD11	1:B:572:ASN:HB3	1.80	0.64
1:B:164:ILE:H	1:B:164:ILE:CD1	2.00	0.63
1:A:555:ALA:HB1	1:A:559:ARG:HH12	1.62	0.63
1:C:120:PRO:HD2	1:C:131:HIS:HE2	1.64	0.63
1:C:330:ARG:O	1:C:333:GLN:HB2	1.97	0.63
1:B:641:PHE:HA	1:B:646:HIS:CD2	2.33	0.63
1:C:465:LYS:NZ	1:C:675:ASN:HD21	1.96	0.63
1:B:76:GLU:HG2	1:B:382:GLN:HE22	1.63	0.63
1:D:116:GLU:HB3	1:D:320:TYR:OH	1.98	0.63
1:A:43:GLU:CD	1:A:43:GLU:N	2.52	0.63
1:D:767:PHE:O	1:D:771:PHE:HB2	1.97	0.63
2:E:4:CTG:H5'	2:E:4:CTG:C6	2.22	0.63
1:C:524:ASP:HA	1:C:527:LYS:CE	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:VAL:O	1:C:271:LEU:HD23	1.99	0.63
1:A:439:LEU:O	1:A:443:ILE:HG13	1.98	0.63
1:C:187:ILE:HG22	1:C:187:ILE:O	1.97	0.63
1:C:642:ARG:CD	1:C:642:ARG:H	2.11	0.63
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.80	0.63
1:B:401:PRO:O	1:B:402:ASN:HB2	1.98	0.63
1:D:125:GLU:HG3	1:D:127:SER:H	1.62	0.63
1:D:171:GLN:OE1	1:D:303:LEU:HD11	1.98	0.63
1:A:708:TYR:CZ	1:A:728:MET:HG3	2.33	0.63
1:B:334:ILE:O	1:B:338:ARG:HG2	1.99	0.63
1:C:382:GLN:HG2	1:C:383:GLY:H	1.61	0.63
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.29	0.63
1:D:189:MET:HB3	1:D:191:PHE:CZ	2.34	0.63
1:C:204:PHE:CE1	1:C:208:LYS:HG3	2.33	0.63
1:D:21:ASP:HB2	1:D:23:ASN:OD1	1.98	0.63
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.79	0.63
1:C:791:TYR:CD2	1:C:802:PRO:HD3	2.34	0.63
1:B:117:VAL:HG21	1:B:225:TYR:CE2	2.34	0.63
1:C:422:GLN:HG3	1:C:678:GLN:O	1.99	0.63
1:D:864:HIS:C	1:D:866:MET:H	2.01	0.63
1:A:559:ARG:HH11	1:A:559:ARG:CG	2.10	0.63
1:A:836:ARG:HG3	1:A:867:ASP:HA	1.80	0.63
1:D:183:ILE:O	1:D:186:ILE:HG12	1.99	0.63
1:A:276:LEU:HD21	1:A:341:ILE:HD13	1.79	0.63
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.34	0.63
2:K:8:DT:H2"	2:K:9:DG:C8	2.34	0.62
1:D:444:ASN:HA	1:D:599:ARG:HH11	1.62	0.62
1:C:6:LEU:HD13	1:C:211:VAL:HG21	1.81	0.62
1:D:219:GLU:OE1	1:D:262:ILE:HD13	1.99	0.62
1:D:605:LEU:HD22	1:D:632:ILE:HD11	1.80	0.62
1:B:740:ALA:HB2	1:B:778:SER:HB2	1.81	0.62
2:G:6:DA:H2"	2:G:7:DA:C5'	2.28	0.62
1:A:239:ALA:O	1:A:242:LEU:HB2	1.99	0.62
3:J:110:DA:H2"	3:J:111:DT:H5'	1.80	0.62
1:D:170:LEU:HD22	1:D:177:GLU:HG2	1.79	0.62
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.15	0.62
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.33	0.62
1:B:470:VAL:O	1:B:474:GLU:HB2	1.99	0.62
1:B:273:TYR:OH	1:B:340:PHE:HB2	2.00	0.62
1:C:787:ASN:HD22	1:C:790:LYS:HD2	1.64	0.62
1:D:713:TRP:CZ3	1:D:723:PRO:HD3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:THR:HG21	1:D:267:GLY:O	2.00	0.62
1:C:167:ALA:O	1:C:176:ASP:HB2	2.00	0.62
1:C:195:LYS:NZ	1:C:195:LYS:N	2.39	0.62
1:B:837:GLU:HG2	1:B:838:GLY:N	2.14	0.62
1:A:810:THR:HG22	1:A:841:PHE:HB3	1.82	0.62
1:A:362:ILE:HD11	1:A:569:ALA:HA	1.81	0.62
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.81	0.62
1:A:467:ARG:HG3	1:A:467:ARG:HH11	1.64	0.62
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.34	0.62
1:C:540:GLU:O	1:C:544:ARG:HG3	2.00	0.62
1:A:499:ILE:HB	1:A:542:LEU:HD13	1.80	0.62
1:D:294:SER:HB3	1:D:300:VAL:HG21	1.80	0.62
1:C:154:SER:C	1:C:156:TYR:H	2.01	0.62
1:D:247:LYS:O	1:D:266:PHE:HB2	1.99	0.62
1:C:839:ASN:OD1	1:C:841:PHE:HB2	1.99	0.62
1:D:90:LEU:HD12	1:D:363:LYS:HE3	1.81	0.62
1:B:468:ASP:N	1:B:468:ASP:OD2	2.33	0.62
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.35	0.62
1:D:725:LEU:H	1:D:725:LEU:HD13	1.65	0.62
1:B:171:GLN:NE2	1:B:303:LEU:HD13	2.15	0.62
1:C:365:TRP:CE2	1:C:566:LEU:HD13	2.34	0.62
1:B:499:ILE:CG1	1:B:542:LEU:HD13	2.30	0.61
1:D:313:ARG:HG3	1:D:317:HIS:HD2	1.65	0.61
2:I:4:CTG:C5'	2:I:4:CTG:H6	2.29	0.61
1:A:218:VAL:HG23	1:A:222:ALA:HB3	1.81	0.61
1:D:736:SER:HA	1:D:782:VAL:HB	1.82	0.61
1:D:750:ARG:HH11	1:D:754:GLN:NE2	1.97	0.61
1:D:707:ARG:HA	1:D:729:GLY:HA3	1.82	0.61
1:B:129:ALA:HB1	1:B:229:ARG:HG2	1.82	0.61
1:B:319:ARG:O	1:B:323:TYR:HB2	2.00	0.61
1:D:811:TYR:CB	1:D:846:ILE:HB	2.30	0.61
1:A:362:ILE:HD13	2:E:3:DT:C5'	2.24	0.61
1:A:656:ARG:HA	1:A:660:GLU:HG3	1.83	0.61
1:B:82:ALA:O	1:B:382:GLN:HB2	2.00	0.61
1:D:576:ARG:HB2	1:D:576:ARG:NH1	2.16	0.61
1:C:97:TYR:O	1:C:352:LYS:HE2	2.00	0.61
3:F:110:DA:H2"	3:F:111:DT:C5'	2.28	0.61
1:D:818:ASN:OD1	1:D:857:LEU:HD12	2.01	0.61
1:B:233:ILE:HD12	1:B:233:ILE:N	2.15	0.61
1:A:745:LEU:HD13	1:A:876:PHE:HD1	1.65	0.61
1:C:455:SER:OG	1:C:676:ASN:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:N	1:A:280:PHE:CD1	2.66	0.61
1:D:198:LEU:HD13	1:D:198:LEU:O	2.00	0.61
1:C:514:LEU:HD21	1:C:526:ILE:HG23	1.82	0.61
1:B:797:PRO:HG3	1:B:806:ARG:HH12	1.65	0.61
1:D:441:ASP:O	1:D:446:VAL:HG12	2.00	0.61
2:G:4:CTG:H6	2:G:4:CTG:C5'	2.31	0.61
1:D:725:LEU:N	1:D:725:LEU:HD13	2.15	0.61
1:C:775:ASN:OD1	1:C:777:ILE:N	2.30	0.61
1:B:685:ARG:HG2	1:B:685:ARG:HH11	1.66	0.61
1:D:575:PHE:HE2	1:D:577:TYR:HB2	1.65	0.61
1:A:840:PRO:C	1:A:842:GLY:H	2.04	0.61
1:A:410:PHE:CD1	1:A:410:PHE:N	2.68	0.61
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.82	0.61
1:D:533:LEU:HD12	1:D:536:LYS:H	1.66	0.61
1:C:135:ALA:O	1:C:136:ILE:HG13	2.01	0.61
1:A:303:LEU:HD12	1:A:323:TYR:CA	2.31	0.61
1:D:779:ILE:CG1	1:D:871:LEU:HD21	2.31	0.61
1:A:276:LEU:CD2	1:A:341:ILE:HD13	2.30	0.61
1:A:153:ASN:ND2	1:A:158:ASN:HB3	2.16	0.61
1:C:195:LYS:HZ3	1:C:195:LYS:HB2	1.64	0.61
1:D:833:LEU:HB2	1:D:848:TRP:HH2	1.65	0.61
1:B:621:ASP:HB3	3:H:114:DA:H5"	1.83	0.61
1:A:408:MET:CE	1:A:655:ALA:HB2	2.31	0.61
1:C:78:ILE:HD11	1:C:80:LEU:HD23	1.82	0.61
1:A:132:PRO:HB3	1:A:194:GLU:OE2	2.01	0.61
1:C:720:TYR:CE1	1:C:724:LYS:HD2	2.36	0.61
1:C:542:LEU:O	1:C:546:GLN:HG3	2.01	0.61
1:D:156:TYR:N	1:D:156:TYR:CD2	2.65	0.61
1:D:508:LEU:HD13	1:D:509:SER:N	2.15	0.60
1:D:403:ARG:HH22	1:D:889:LEU:HD21	1.64	0.60
1:C:642:ARG:HE	1:C:646:HIS:HD2	1.39	0.60
1:C:642:ARG:HH11	1:C:646:HIS:HB3	1.65	0.60
1:B:504:HIS:O	1:B:506:PRO:HD3	2.01	0.60
1:A:836:ARG:HG3	1:A:867:ASP:CA	2.31	0.60
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.82	0.60
3:H:110:DA:H2"	3:H:111:DT:H5'	1.83	0.60
1:B:365:TRP:CD2	1:B:566:LEU:HD13	2.36	0.60
2:G:10:DA:H2"	2:G:11:DC:C5'	2.31	0.60
2:G:16:DG:H2"	2:G:17:DC:C5'	2.32	0.60
3:F:104:DG:C3'	3:F:105:DC:H5"	2.31	0.60
1:D:833:LEU:HB2	1:D:848:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.16	0.60
1:D:216:TRP:HB2	1:D:290:LEU:HD12	1.83	0.60
1:C:203:ASN:O	1:C:207:GLN:HG2	2.01	0.60
1:A:772:ARG:HD2	1:A:868:TYR:CD2	2.36	0.60
1:A:38:PHE:CD2	1:A:59:ARG:HA	2.36	0.60
1:D:191:PHE:HD1	1:D:197:LEU:HD23	1.65	0.60
1:B:629:ALA:HA	1:B:632:ILE:HG12	1.82	0.60
1:D:191:PHE:CD1	1:D:197:LEU:HD23	2.35	0.60
1:B:126:PRO:HG3	1:B:221:PHE:HD1	1.66	0.60
1:D:469:GLY:C	1:D:472:PRO:HD2	2.22	0.60
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.67	0.60
1:C:151:LEU:HD21	1:C:154:SER:HB3	1.83	0.60
1:A:725:LEU:HD11	1:A:750:ARG:HB2	1.82	0.60
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.83	0.60
1:A:783:SER:HA	3:F:111:DT:OP1	2.01	0.60
2:K:10:DA:H2"	2:K:11:DC:C5'	2.31	0.60
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.67	0.60
1:B:288:TYR:CD1	1:B:293:ILE:HD11	2.37	0.60
1:C:822:PRO:HD2	1:C:855:THR:OG1	2.01	0.60
1:C:73:LYS:HB3	1:C:73:LYS:HZ3	1.67	0.60
1:C:327:ALA:O	1:C:330:ARG:HB2	2.01	0.60
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.84	0.60
1:A:194:GLU:OE1	1:A:229:ARG:NH1	2.34	0.59
1:D:231:LYS:O	1:D:235:GLY:HA2	2.02	0.59
1:A:813:ARG:HB2	1:A:813:ARG:HH11	1.67	0.59
1:A:137:THR:HB	1:A:328:VAL:HG21	1.83	0.59
1:A:862:VAL:C	1:A:864:HIS:H	2.04	0.59
1:B:505:ASN:ND2	1:B:507:ASN:ND2	2.46	0.59
1:D:194:GLU:O	1:D:198:LEU:HB2	2.02	0.59
1:A:855:THR:HG22	1:A:857:LEU:HG	1.83	0.59
1:D:835:LEU:CD2	1:D:846:ILE:HG23	2.33	0.59
1:D:159:VAL:HG11	1:D:317:HIS:CG	2.37	0.59
1:B:777:ILE:HD11	1:B:853:GLU:CG	2.31	0.59
1:A:482:ARG:HE	1:A:556:GLN:NE2	2.00	0.59
1:C:302:LYS:HD3	1:C:303:LEU:N	2.17	0.59
1:B:102:LYS:HD2	1:B:103:TYR:N	2.18	0.59
1:B:706:LYS:HD2	3:H:113:DC:H1'	1.84	0.59
1:D:503:LEU:O	1:D:503:LEU:HD23	2.03	0.59
1:A:514:LEU:HD13	1:A:529:LYS:HZ3	1.68	0.59
1:A:132:PRO:HA	1:A:229:ARG:NH1	2.17	0.59
1:D:136:ILE:HG23	1:D:149:PHE:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ALA:O	1:D:71:TRP:HB3	2.02	0.59
2:I:10:DA:H2"	2:I:11:DC:C5'	2.32	0.59
1:A:839:ASN:HB2	1:A:840:PRO:CD	2.22	0.59
1:B:642:ARG:H	1:B:646:HIS:HD2	1.50	0.59
1:D:171:GLN:HE22	1:D:303:LEU:CD1	2.15	0.59
1:D:305:TYR:OH	1:D:309:ILE:HA	2.03	0.59
1:D:542:LEU:HD11	1:D:546:GLN:HE21	1.67	0.59
1:A:279:LYS:HD3	1:A:359:PHE:HD1	1.68	0.59
1:D:286:PRO:HB3	1:D:782:VAL:HG11	1.83	0.59
1:A:807:GLY:HA2	1:A:845:CYS:O	2.03	0.59
1:D:598:GLU:HG3	1:D:617:VAL:HG21	1.83	0.59
1:A:811:TYR:CZ	1:A:815:ILE:HD13	2.38	0.59
1:D:777:ILE:HG23	1:D:831:TYR:CE1	2.37	0.59
1:A:290:LEU:O	1:A:294:SER:HB2	2.03	0.59
1:D:132:PRO:HA	1:D:229:ARG:NH2	2.18	0.59
1:C:170:LEU:HA	1:C:177:GLU:HG2	1.85	0.59
1:D:335:ASP:O	1:D:339:GLN:N	2.32	0.59
1:C:277:TYR:O	1:C:281:SER:HB3	2.03	0.59
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.84	0.59
1:D:77:ASP:O	1:D:78:ILE:HD13	2.03	0.58
1:A:298:LEU:N	1:A:298:LEU:HD12	2.17	0.58
1:B:471:VAL:HG11	1:B:570:LEU:HD11	1.85	0.58
1:B:505:ASN:HD22	1:B:507:ASN:ND2	2.01	0.58
1:A:40:HIS:CD2	1:A:57:CYS:SG	2.95	0.58
1:C:274:ILE:HG23	1:C:275:ASP:N	2.17	0.58
1:D:770:GLU:O	1:D:774:LEU:HG	2.03	0.58
1:D:594:LEU:HD11	1:D:625:ILE:HG22	1.86	0.58
1:D:779:ILE:HG13	1:D:871:LEU:HD21	1.84	0.58
1:D:777:ILE:HG23	1:D:831:TYR:HE1	1.68	0.58
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.38	0.58
1:D:285:GLN:HE21	1:D:285:GLN:H	1.52	0.58
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.85	0.58
1:D:848:TRP:CG	1:D:854:ILE:HB	2.38	0.58
3:J:111:DT:H2"	3:J:112:DT:H5"	1.85	0.58
1:D:381:PRO:O	1:D:576:ARG:HD2	2.03	0.58
1:C:42:PRO:HG2	1:C:45:GLN:HG3	1.84	0.58
1:B:425:ILE:HG23	1:B:463:TYR:CE2	2.39	0.58
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.38	0.58
1:D:197:LEU:O	1:D:197:LEU:HD22	2.04	0.58
1:B:83:LEU:CD1	1:B:83:LEU:H	2.14	0.58
1:B:664:ASP:OD2	1:B:668:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ILE:HG22	1:B:373:LEU:CD1	2.32	0.58
1:B:408:MET:HE2	1:B:685:ARG:HD3	1.86	0.58
1:B:204:PHE:CE1	1:B:208:LYS:HD2	2.37	0.58
1:A:743:LYS:O	1:A:746:LYS:HB3	2.04	0.58
1:D:397:LYS:O	1:D:399:PRO:HD3	2.02	0.58
1:A:120:PRO:HG2	1:A:156:TYR:CE1	2.39	0.58
1:A:364:THR:O	1:A:368:ILE:HG13	2.03	0.58
1:A:494:ARG:NH2	1:A:521:ASP:HB3	2.18	0.58
1:D:786:ASN:HB2	3:L:110:DA:OP1	2.04	0.58
1:D:82:ALA:H	1:D:382:GLN:HE21	1.50	0.58
1:A:467:ARG:HG3	1:A:467:ARG:NH1	2.18	0.58
1:B:739:LYS:HE2	1:B:742:GLN:HE22	1.66	0.58
1:C:788:ILE:HG13	1:C:826:GLU:OE1	2.04	0.58
1:B:217:ASN:OD1	1:B:274:ILE:CD1	2.51	0.58
1:C:137:THR:HG21	1:C:325:ILE:HA	1.85	0.58
1:D:9:GLU:HG3	1:D:267:GLY:H	1.69	0.58
1:A:685:ARG:NH2	1:A:717:GLY:H	2.01	0.58
1:A:779:ILE:O	1:A:779:ILE:HG13	2.03	0.58
1:A:236:GLU:CG	1:A:240:LYS:HE2	2.30	0.58
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.38	0.58
1:C:465:LYS:HZ3	1:C:675:ASN:HD21	1.52	0.58
3:H:102:DC:H2"	3:H:103:DG:OP2	2.04	0.58
1:B:317:HIS:O	1:B:320:TYR:HB3	2.04	0.58
1:C:831:TYR:CD2	1:C:850:SER:HA	2.38	0.57
1:D:305:TYR:CE2	1:D:312:LEU:HD13	2.39	0.57
1:D:132:PRO:HA	1:D:229:ARG:HH21	1.68	0.57
1:A:42:PRO:HG2	1:A:45:GLN:HB2	1.86	0.57
1:A:523:SER:O	1:A:527:LYS:HB3	2.04	0.57
1:B:16:PHE:HB3	1:B:245:HIS:CE1	2.40	0.57
1:D:229:ARG:HH11	1:D:233:ILE:HD11	1.68	0.57
1:A:708:TYR:CE2	1:A:728:MET:CG	2.85	0.57
2:I:4:CTG:O6	2:I:4:CTG:H5"	2.03	0.57
1:B:117:VAL:CG2	1:B:133:ILE:HG12	2.34	0.57
1:B:855:THR:HG21	1:B:857:LEU:HD12	1.86	0.57
1:C:193:ASN:HD22	1:C:195:LYS:HZ1	1.51	0.57
1:D:313:ARG:HG3	1:D:317:HIS:CD2	2.40	0.57
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.34	0.57
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.16	0.57
1:A:405:LYS:O	1:A:690:GLY:HA2	2.04	0.57
1:D:810:THR:HG22	1:D:846:ILE:HG22	1.85	0.57
1:D:150:ASP:HB3	1:D:188:TYR:CE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ILE:HG13	1:D:15:ILE:O	2.04	0.57
1:D:347:MET:HG2	1:D:358:VAL:HG13	1.87	0.57
1:C:183:ILE:HD12	1:C:186:ILE:CD1	2.33	0.57
1:C:726:LYS:CG	1:C:728:MET:HE3	2.33	0.57
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.39	0.57
1:D:518:TYR:CD1	1:D:518:TYR:N	2.73	0.57
1:D:503:LEU:HG	1:D:535:ALA:HB2	1.85	0.57
1:C:231:LYS:O	1:C:231:LYS:HD2	2.05	0.57
1:A:839:ASN:CB	1:A:840:PRO:HD2	2.22	0.57
1:B:273:TYR:HA	1:B:276:LEU:HB2	1.87	0.57
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.40	0.57
1:D:290:LEU:O	1:D:290:LEU:HD23	2.04	0.57
1:A:109:ARG:NH1	1:A:140:ASP:OD2	2.37	0.57
1:D:214:THR:O	1:D:218:VAL:HG21	2.04	0.57
1:D:365:TRP:CE2	1:D:566:LEU:HD13	2.40	0.57
1:B:835:LEU:HD21	1:B:862:VAL:HG13	1.85	0.57
1:C:465:LYS:NZ	1:C:675:ASN:ND2	2.53	0.57
1:B:210:PRO:HG2	1:B:213:LEU:HD13	1.86	0.57
1:D:295:GLU:OE1	1:D:302:LYS:HG3	2.05	0.57
1:A:602:ASN:ND2	1:A:616:PHE:HB2	2.20	0.57
1:B:221:PHE:C	1:B:224:PRO:HD2	2.25	0.57
1:C:811:TYR:HA	1:C:846:ILE:HD11	1.86	0.57
1:B:642:ARG:H	1:B:646:HIS:CD2	2.23	0.57
1:D:285:GLN:NE2	1:D:285:GLN:H	2.02	0.57
1:B:342:ASN:HB2	4:B:923:HOH:O	2.05	0.57
1:D:249:ARG:O	1:D:264:THR:HG22	2.05	0.57
1:D:534:SER:O	1:D:538:LEU:HD13	2.05	0.57
1:D:214:THR:HG21	1:D:273:TYR:HD2	1.69	0.57
1:D:405:LYS:O	1:D:690:GLY:HA2	2.05	0.57
1:C:124:PRO:HB2	1:C:225:TYR:HE2	1.68	0.57
1:A:395:PHE:HA	4:A:942:HOH:O	2.03	0.57
1:A:862:VAL:O	1:A:865:TRP:N	2.36	0.57
3:F:109:DC:H1'	3:F:110:DA:H5"	1.87	0.57
1:A:37:LEU:HD11	1:A:72:ILE:HD11	1.86	0.57
3:L:101:DG:H2"	3:L:102:DC:C6	2.40	0.57
1:A:654:PHE:HE1	1:A:659:MET:HG3	1.69	0.57
1:A:129:ALA:HA	1:A:225:TYR:CZ	2.39	0.57
1:A:66:ARG:O	1:A:70:GLN:HB2	2.04	0.57
1:D:270:VAL:O	1:D:271:LEU:HD23	2.05	0.56
1:A:824:VAL:HG11	1:A:830:VAL:HG12	1.87	0.56
1:B:858:ILE:O	1:B:862:VAL:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:CE	1:B:350:TYR:HD2	2.18	0.56
1:B:117:VAL:HG13	1:B:132:PRO:O	2.05	0.56
1:D:101:ILE:HG22	1:D:102:LYS:N	2.20	0.56
1:D:546:GLN:HA	1:D:549:GLU:HB3	1.87	0.56
1:B:505:ASN:HB3	1:B:535:ALA:CB	2.35	0.56
1:D:229:ARG:HH11	1:D:229:ARG:HG2	1.69	0.56
1:D:305:TYR:HE2	1:D:312:LEU:HD13	1.70	0.56
1:C:149:PHE:O	1:C:197:LEU:HD11	2.05	0.56
2:G:15:DC:H6	2:G:15:DC:H5'	1.70	0.56
1:A:514:LEU:CD2	1:A:529:LYS:HE2	2.36	0.56
1:D:376:GLN:HB2	1:D:378:LYS:HG2	1.85	0.56
1:A:654:PHE:CE1	1:A:659:MET:HG3	2.41	0.56
3:J:110:DA:H1'	3:J:111:DT:H5"	1.87	0.56
1:A:876:PHE:O	1:A:879:PRO:HG2	2.04	0.56
1:D:575:PHE:CE2	1:D:577:TYR:HB2	2.39	0.56
1:A:411:ASP:OD1	1:A:686:GLU:HG3	2.06	0.56
1:B:376:GLN:NE2	1:B:378:LYS:NZ	2.52	0.56
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.85	0.56
1:D:202:LEU:HD21	1:D:241:ARG:CD	2.18	0.56
1:D:810:THR:CG2	1:D:846:ILE:HG22	2.36	0.56
3:F:110:DA:H1'	3:F:111:DT:H5"	1.87	0.56
1:C:686:GLU:HG3	1:C:715:MET:HE1	1.86	0.56
1:B:159:VAL:HG11	1:B:313:ARG:O	2.05	0.56
1:D:89:LYS:O	1:D:93:LEU:HD13	2.05	0.56
1:C:451:SER:OG	1:C:453:VAL:HG22	2.05	0.56
1:B:821:ALA:HB1	1:B:822:PRO:HD2	1.87	0.56
1:C:139:TYR:CE2	1:C:332:LEU:HD21	2.41	0.56
2:G:6:DA:H2"	2:G:7:DA:H5'	1.87	0.56
1:C:731:GLU:HA	1:C:734:LYS:HG3	1.88	0.56
1:D:878:LYS:O	1:D:881:GLU:HB2	2.06	0.56
1:D:213:LEU:HD22	1:D:218:VAL:HG11	1.87	0.56
1:C:316:ASN:OD1	1:C:318:GLN:HB3	2.06	0.56
1:D:552:GLY:O	1:D:556:GLN:HB3	2.06	0.56
1:B:863:LEU:HA	1:B:866:MET:HE3	1.87	0.56
1:B:166:ILE:N	1:B:166:ILE:HD12	2.18	0.56
1:D:264:THR:O	1:D:264:THR:HG23	2.06	0.56
1:C:9:GLU:OE2	1:C:266:PHE:HA	2.05	0.56
1:A:509:SER:H	1:A:534:SER:HB3	1.71	0.56
1:A:509:SER:N	1:A:534:SER:HB3	2.19	0.56
1:C:461:MET:SD	1:C:581:ARG:HD2	2.45	0.56
1:B:738:PRO:HB2	1:B:741:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLN:O	1:A:484:GLU:HB3	2.05	0.56
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.70	0.56
3:J:105:DC:H2'	3:J:106:DT:C7	2.35	0.56
1:B:85:MET:HE2	1:B:87:ASP:N	2.01	0.56
1:D:365:TRP:HA	1:D:368:ILE:HD12	1.87	0.56
1:C:380:ILE:HD12	1:C:576:ARG:CZ	2.35	0.56
1:A:399:PRO:HG2	1:A:704:GLY:HA2	1.87	0.56
1:C:189:MET:O	1:C:191:PHE:CE1	2.59	0.56
1:C:475:ILE:HG23	1:C:476:THR:N	2.20	0.56
1:C:506:PRO:HB3	1:C:535:ALA:HB2	1.87	0.56
1:B:644:THR:HG23	1:B:645:ASN:N	2.21	0.56
1:A:246:ARG:NH1	1:A:246:ARG:HG2	2.20	0.56
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.88	0.56
1:D:442:TYR:HB3	1:D:592:MET:CE	2.34	0.56
1:D:830:VAL:HA	1:D:850:SER:HB3	1.88	0.56
1:A:4:PHE:CD1	1:A:4:PHE:N	2.74	0.56
1:C:642:ARG:HE	1:C:646:HIS:CG	2.19	0.56
3:J:105:DC:H5'	3:J:105:DC:H6	1.71	0.56
1:D:132:PRO:HA	1:D:229:ARG:CZ	2.35	0.56
1:D:154:SER:HB2	1:D:313:ARG:NH1	2.20	0.56
1:A:653:LYS:HD3	1:A:657:GLU:OE1	2.06	0.56
1:D:777:ILE:O	1:D:777:ILE:CG2	2.53	0.56
1:C:720:TYR:CZ	1:C:724:LYS:HD2	2.40	0.56
1:D:419:ILE:HD13	1:D:589:PHE:HD1	1.69	0.56
1:D:453:VAL:HG23	1:D:454:TYR:CD1	2.40	0.56
1:D:151:LEU:HD13	1:D:151:LEU:C	2.27	0.56
1:B:270:VAL:C	1:B:271:LEU:HD12	2.26	0.56
1:C:154:SER:O	1:C:156:TYR:N	2.39	0.56
1:A:4:PHE:O	1:A:19:TYR:HB2	2.05	0.56
3:J:105:DC:H6	3:J:105:DC:C5'	2.19	0.55
1:A:501:GLU:HA	1:A:504:HIS:CE1	2.41	0.55
1:A:880:LEU:O	1:A:883:PHE:HB2	2.05	0.55
1:D:402:ASN:CG	1:D:403:ARG:H	2.09	0.55
1:D:554:THR:O	1:D:558:ASN:HB2	2.06	0.55
1:D:455:SER:HA	1:D:675:ASN:O	2.06	0.55
1:D:131:HIS:O	1:D:229:ARG:NE	2.39	0.55
1:C:214:THR:HG21	1:C:341:ILE:HD11	1.88	0.55
1:A:686:GLU:O	1:A:716:GLU:N	2.33	0.55
1:A:19:TYR:HE1	1:A:29:ARG:HG2	1.71	0.55
1:D:48:LYS:O	1:D:377:ASN:HB3	2.06	0.55
1:D:513:PRO:HA	1:D:541:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:HH21	1:D:208:LYS:CB	2.19	0.55
1:A:279:LYS:HZ2	2:E:3:DT:H71	1.71	0.55
1:B:516:VAL:CG1	1:B:544:ARG:HH11	2.18	0.55
1:A:489:MET:SD	1:A:553:MET:HG2	2.46	0.55
1:D:516:VAL:HG12	1:D:517:ASP:N	2.21	0.55
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.42	0.55
1:A:362:ILE:HD11	1:A:572:ASN:HD22	1.70	0.55
1:B:668:ARG:HH11	1:B:668:ARG:CG	2.14	0.55
1:D:412:LEU:HD21	1:D:683:MET:HE3	1.87	0.55
1:A:113:PHE:CE1	1:A:218:VAL:HG21	2.42	0.55
1:C:499:ILE:CG2	1:C:542:LEU:HB2	2.37	0.55
1:A:211:VAL:HG12	1:A:212:ILE:HG12	1.89	0.55
1:B:113:PHE:HB2	1:B:137:THR:O	2.07	0.55
1:A:781:SER:O	1:A:831:TYR:HA	2.06	0.55
1:C:791:TYR:HD2	1:C:801:CYS:HA	1.68	0.55
1:B:129:ALA:HB1	1:B:229:ARG:CD	2.36	0.55
1:D:741:VAL:HG12	1:D:745:LEU:HG	1.88	0.55
1:C:37:LEU:C	1:C:38:PHE:CD1	2.80	0.55
1:A:347:MET:HE3	1:A:347:MET:HA	1.87	0.55
1:B:145:ARG:HG3	1:B:185:LYS:O	2.07	0.55
1:D:824:VAL:HG23	1:D:830:VAL:HG11	1.87	0.55
1:B:796:PHE:CD1	1:B:813:ARG:NH1	2.74	0.55
1:A:597:ILE:HG12	1:A:667:PHE:CE2	2.41	0.55
1:C:528:GLU:HA	1:C:528:GLU:OE2	2.07	0.55
1:B:115:ILE:HD13	1:B:115:ILE:H	1.71	0.55
2:G:10:DA:H2"	2:G:11:DC:H5"	1.89	0.55
1:A:604:TYR:O	1:A:608:VAL:HG22	2.07	0.55
1:B:147:TYR:CD1	1:B:147:TYR:N	2.75	0.55
1:B:20:ILE:HG22	1:B:24:GLY:HA2	1.87	0.55
1:B:772:ARG:NH2	1:B:868:TYR:HB2	2.21	0.55
1:A:414:SER:O	1:A:417:PRO:HD2	2.07	0.55
1:C:10:GLN:HG3	1:C:65:MET:HE1	1.87	0.55
1:C:251:LYS:HB3	1:C:262:ILE:HG13	1.87	0.55
1:B:3:GLU:HG2	1:B:21:ASP:HA	1.89	0.55
1:D:814:ALA:HB3	1:D:841:PHE:CD1	2.41	0.55
1:A:846:ILE:HD12	1:A:847:ALA:O	2.07	0.55
1:D:159:VAL:HG21	1:D:317:HIS:CD2	2.42	0.55
2:E:16:DG:N2	3:F:103:DG:N2	2.54	0.55
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.36	0.55
1:D:52:ILE:CG2	1:D:381:PRO:HD3	2.37	0.55
1:C:202:LEU:HD23	1:C:241:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:ASP:HA	1:B:809:LEU:HD21	1.87	0.55
1:A:420:ILE:HG12	1:A:586:ILE:HD11	1.87	0.55
1:B:878:LYS:O	1:B:878:LYS:HD3	2.06	0.55
1:C:41:CYS:CB	1:C:58:THR:HG22	2.25	0.55
1:B:347:MET:HE3	1:B:350:TYR:HD2	1.72	0.55
1:D:395:PHE:HB3	1:D:594:LEU:HD23	1.89	0.55
1:C:81:GLU:HG2	1:C:83:LEU:CD2	2.36	0.55
2:G:15:DC:H2"	2:G:16:DG:O5'	2.06	0.55
1:A:782:VAL:HG22	1:A:831:TYR:HD1	1.71	0.55
1:A:782:VAL:HG12	1:A:783:SER:N	2.22	0.55
1:B:182:ILE:O	1:B:186:ILE:HG13	2.07	0.55
2:I:12:DA:H2"	2:I:13:DG:H5'	1.89	0.54
1:C:195:LYS:CB	1:C:195:LYS:HZ3	2.21	0.54
1:C:392:PRO:HG2	1:C:584:THR:HG23	1.89	0.54
1:C:111:ALA:HB3	1:C:210:PRO:HB3	1.89	0.54
1:B:145:ARG:HB3	1:B:147:TYR:CE1	2.41	0.54
1:B:504:HIS:C	1:B:506:PRO:HD3	2.28	0.54
1:A:517:ASP:OD1	1:A:519:ARG:HB2	2.06	0.54
1:D:512:GLU:CB	1:D:513:PRO:CA	2.85	0.54
1:D:530:ILE:O	1:D:532:LYS:N	2.40	0.54
3:F:107:DG:H2"	3:F:108:DT:OP2	2.06	0.54
1:A:702:TRP:CD1	1:A:708:TYR:HB3	2.42	0.54
1:D:216:TRP:CH2	1:D:293:ILE:HG12	2.41	0.54
1:D:514:LEU:HD11	1:D:532:LYS:CB	2.37	0.54
1:B:621:ASP:HB3	3:H:114:DA:C5'	2.36	0.54
1:B:116:GLU:N	1:B:135:ALA:O	2.39	0.54
1:B:898:PHE:HD1	1:B:898:PHE:H	1.55	0.54
1:A:4:PHE:CE2	1:A:103:TYR:HB2	2.42	0.54
1:D:450:PRO:HB2	1:D:456:CYS:SG	2.48	0.54
1:D:482:ARG:C	1:D:484:GLU:H	2.11	0.54
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.17	0.54
1:C:147:TYR:HB3	1:C:149:PHE:CE1	2.42	0.54
1:A:41:CYS:HB3	1:A:58:THR:HG22	1.89	0.54
1:D:514:LEU:HD12	1:D:514:LEU:N	2.22	0.54
1:A:798:GLY:N	1:A:801:CYS:SG	2.80	0.54
1:C:143:ASP:O	1:C:144:ASP:HB3	2.07	0.54
1:B:421:ARG:NH1	1:B:421:ARG:HG2	2.23	0.54
1:D:750:ARG:NH1	1:D:754:GLN:NE2	2.55	0.54
1:C:738:PRO:HG2	1:C:741:VAL:CG2	2.37	0.54
1:A:279:LYS:HE3	1:A:280:PHE:CE1	2.42	0.54
1:A:835:LEU:HD21	1:A:846:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:HB2	1:B:591:GLN:NE2	2.11	0.54
1:A:708:TYR:C	1:A:708:TYR:CD2	2.81	0.54
1:D:848:TRP:HB2	1:D:849:PRO:HD2	1.88	0.54
2:G:12:DA:H2"	2:G:13:DG:O5'	2.08	0.54
1:A:395:PHE:HB2	1:A:591:GLN:OE1	2.08	0.54
1:B:836:ARG:NH2	1:B:864:HIS:O	2.41	0.54
1:C:375:GLU:HA	1:C:375:GLU:OE2	2.08	0.54
1:A:362:ILE:CD1	1:A:569:ALA:HA	2.37	0.54
1:A:782:VAL:HG22	1:A:831:TYR:CD1	2.43	0.54
1:A:373:LEU:HD11	1:A:470:VAL:HG11	1.90	0.54
1:D:600:LYS:HE3	1:D:669:GLU:OE2	2.08	0.54
1:C:412:LEU:HG	1:C:683:MET:CE	2.38	0.54
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.23	0.54
1:D:13:ASP:HB3	1:D:64:ASN:HB2	1.88	0.54
1:B:361:PRO:HB3	1:B:565:SER:HB2	1.89	0.54
1:C:685:ARG:HD2	1:C:685:ARG:C	2.28	0.54
1:D:312:LEU:HG	1:D:320:TYR:HB2	1.90	0.54
1:A:835:LEU:HD11	1:A:846:ILE:CG2	2.29	0.54
1:C:215:GLY:HA3	1:C:218:VAL:CG2	2.37	0.54
1:B:609:CYS:HA	1:B:635:LYS:HE3	1.90	0.54
1:C:135:ALA:O	1:C:136:ILE:CG1	2.56	0.54
1:C:836:ARG:HH11	1:C:836:ARG:HG3	1.73	0.54
1:D:856:ASP:HA	1:D:859:LYS:CB	2.38	0.54
1:A:408:MET:HG2	1:A:688:ILE:HG12	1.90	0.54
1:B:353:ILE:HG13	1:B:354:GLN:O	2.07	0.54
1:A:897:LEU:H	1:A:897:LEU:CD1	2.16	0.54
1:C:373:LEU:HD22	1:C:378:LYS:HD2	1.88	0.54
1:B:118:THR:OG1	1:B:313:ARG:HD2	2.07	0.54
1:D:488:TYR:HD1	1:D:519:ARG:HH21	1.56	0.54
1:D:286:PRO:O	1:D:829:LYS:HD3	2.08	0.54
1:B:629:ALA:CA	1:B:632:ILE:HG12	2.38	0.54
1:C:453:VAL:HG23	1:C:454:TYR:N	2.23	0.54
1:C:181:GLU:H	1:C:181:GLU:CD	2.11	0.54
1:D:140:ASP:CB	1:D:143:ASP:HB3	2.35	0.53
1:D:368:ILE:CD1	1:D:562:LEU:HD11	2.39	0.53
1:C:686:GLU:HG3	1:C:715:MET:HE3	1.88	0.53
1:C:154:SER:C	1:C:156:TYR:N	2.61	0.53
1:B:112:ASN:O	1:B:113:PHE:HB3	2.08	0.53
1:B:120:PRO:HG2	1:B:156:TYR:CE2	2.43	0.53
1:D:697:GLY:HA3	1:D:753:LEU:O	2.07	0.53
1:B:273:TYR:O	1:B:277:TYR:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:VAL:HG12	1:D:301:GLY:N	2.23	0.53
1:D:156:TYR:N	1:D:156:TYR:HD2	2.05	0.53
1:D:285:GLN:NE2	1:D:285:GLN:N	2.56	0.53
1:A:108:ILE:HG23	1:A:211:VAL:HG11	1.89	0.53
1:C:215:GLY:HA3	1:C:218:VAL:HG21	1.90	0.53
1:A:668:ARG:O	1:A:672:GLU:HG3	2.09	0.53
1:D:807:GLY:HA2	1:D:845:CYS:O	2.07	0.53
1:C:825:VAL:HB	1:C:828:GLU:CD	2.28	0.53
3:L:101:DG:H2"	3:L:102:DC:C5	2.42	0.53
3:H:106:DT:H2"	3:H:107:DG:O5'	2.07	0.53
1:C:109:ARG:HG2	1:C:210:PRO:HA	1.91	0.53
1:B:177:GLU:HG2	1:B:303:LEU:HD11	1.90	0.53
1:D:20:ILE:HD13	1:D:26:GLU:HA	1.90	0.53
1:D:883:PHE:N	1:D:883:PHE:CD2	2.76	0.53
1:B:216:TRP:CH2	1:B:293:ILE:HG21	2.43	0.53
1:B:516:VAL:HG22	1:B:517:ASP:N	2.22	0.53
2:G:14:DC:H2"	2:G:15:DC:C5'	2.38	0.53
1:C:71:TRP:O	1:C:75:MET:HG2	2.07	0.53
1:B:831:TYR:CE2	1:B:850:SER:HA	2.43	0.53
1:C:163:SER:OG	1:C:166:ILE:HG13	2.09	0.53
2:G:3:DT:H2"	2:G:4:CTG:OP2	2.08	0.53
1:B:147:TYR:H	1:B:147:TYR:HD1	1.56	0.53
1:C:35:PRO:HD3	1:C:65:MET:HG2	1.91	0.53
1:C:362:ILE:HD12	1:C:575:PHE:HB2	1.89	0.53
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.44	0.53
1:D:839:ASN:HD22	1:D:839:ASN:N	2.04	0.53
1:A:279:LYS:NZ	2:E:3:DT:H71	2.24	0.53
1:D:271:LEU:HB3	1:D:276:LEU:HD11	1.91	0.53
1:C:163:SER:CB	1:C:166:ILE:HD12	2.39	0.53
1:D:617:VAL:O	1:D:617:VAL:HG23	2.09	0.53
1:A:347:MET:HA	1:A:347:MET:CE	2.38	0.53
1:D:825:VAL:HB	1:D:828:GLU:CG	2.38	0.53
1:A:776:TYR:CZ	1:A:777:ILE:HG13	2.43	0.53
1:A:313:ARG:O	1:A:317:HIS:HB2	2.09	0.53
1:D:305:TYR:HE1	1:D:309:ILE:HG22	1.74	0.53
1:D:815:ILE:CG2	1:D:858:ILE:HG21	2.26	0.53
1:D:864:HIS:O	1:D:866:MET:N	2.36	0.53
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.08	0.53
1:A:509:SER:H	1:A:534:SER:CB	2.22	0.53
1:A:693:LEU:HD12	1:A:694:GLY:N	2.23	0.53
1:B:597:ILE:HD13	1:B:667:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:DT:C2'	2:G:9:DG:C8	2.92	0.53
1:B:825:VAL:HB	1:B:828:GLU:HG3	1.91	0.53
1:B:456:CYS:SG	1:B:462:MET:HG2	2.49	0.53
1:B:811:TYR:HH	1:B:822:PRO:HG2	1.71	0.53
1:D:668:ARG:HG3	1:D:679:HIS:CE1	2.43	0.53
1:A:48:LYS:HE3	1:A:377:ASN:OD1	2.09	0.53
1:A:840:PRO:O	1:A:842:GLY:N	2.41	0.53
1:A:153:ASN:HD22	1:A:158:ASN:HB3	1.73	0.53
1:D:485:HIS:HB3	1:D:556:GLN:CB	2.39	0.53
1:D:8:VAL:HG11	1:D:93:LEU:HD11	1.91	0.53
1:D:546:GLN:O	1:D:550:VAL:HG23	2.09	0.53
1:A:362:ILE:HG12	1:A:572:ASN:HD22	1.74	0.53
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.90	0.53
1:C:686:GLU:OE1	1:C:716:GLU:HG3	2.09	0.53
1:D:738:PRO:HB2	1:D:778:SER:O	2.08	0.53
1:A:706:LYS:CE	3:F:113:DC:O2	2.56	0.53
1:D:147:TYR:CE2	1:D:187:ILE:HD13	2.44	0.53
1:C:195:LYS:HZ2	1:C:195:LYS:H	1.50	0.52
1:A:789:ALA:O	1:A:791:TYR:N	2.42	0.52
1:B:186:ILE:O	1:B:187:ILE:HG13	2.09	0.52
1:A:485:HIS:C	1:A:487:GLY:N	2.59	0.52
1:D:416:TYR:HD2	1:D:586:ILE:CG2	2.22	0.52
1:C:645:ASN:OD1	1:C:719:ARG:NH1	2.40	0.52
1:A:622:THR:HG22	1:A:623:ASP:N	2.24	0.52
1:A:612:GLU:HG2	1:A:612:GLU:O	2.09	0.52
1:C:855:THR:HG22	1:C:857:LEU:N	2.19	0.52
1:C:119:SER:HA	1:C:131:HIS:CD2	2.43	0.52
1:A:422:GLN:HE21	1:A:680:LEU:H	1.54	0.52
1:B:747:GLU:HG2	1:B:763:TYR:CZ	2.44	0.52
1:C:204:PHE:HE1	1:C:208:LYS:HG3	1.74	0.52
1:B:159:VAL:HG22	1:B:313:ARG:HH22	1.75	0.52
1:A:516:VAL:HG21	1:A:522:PHE:CE2	2.44	0.52
1:D:114:ASP:CB	1:D:328:VAL:HG13	2.39	0.52
1:A:625:ILE:HG13	1:A:625:ILE:O	2.08	0.52
1:B:218:VAL:HG12	1:B:223:ILE:HD11	1.91	0.52
1:B:162:TRP:HA	1:B:318:GLN:NE2	2.20	0.52
1:B:117:VAL:HG22	1:B:132:PRO:O	2.10	0.52
1:A:855:THR:CG2	1:A:857:LEU:HG	2.39	0.52
1:B:11:ILE:HD12	1:B:16:PHE:CD1	2.44	0.52
1:B:810:THR:HG23	1:B:813:ARG:HH21	1.74	0.52
1:C:493:GLN:HG3	1:C:549:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:ALA:HB1	1:B:889:LEU:HD12	1.91	0.52
1:D:543:PHE:O	1:D:547:ARG:HB3	2.10	0.52
1:C:231:LYS:C	1:C:231:LYS:HE2	2.29	0.52
1:A:804:HIS:HE2	3:F:110:DA:P	2.32	0.52
1:B:229:ARG:O	1:B:233:ILE:HD13	2.09	0.52
1:C:412:LEU:HD13	1:C:415:LEU:CD1	2.39	0.52
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.22	0.52
1:A:727:ILE:HD13	1:A:749:ILE:HD12	1.90	0.52
1:D:403:ARG:NH2	1:D:889:LEU:HD21	2.24	0.52
1:B:206:GLN:HE22	1:B:246:ARG:HH22	1.58	0.52
1:A:471:VAL:HB	1:A:472:PRO:CD	2.38	0.52
1:A:824:VAL:CG1	1:A:849:PRO:HG3	2.39	0.52
1:B:499:ILE:CD1	1:B:499:ILE:H	2.04	0.52
1:D:686:GLU:HB3	1:D:715:MET:HE1	1.91	0.52
1:D:191:PHE:HB2	1:D:197:LEU:HB2	1.92	0.52
1:A:153:ASN:HB3	1:A:158:ASN:HD22	1.74	0.52
2:K:6:DA:H2"	2:K:7:DA:H5'	1.91	0.52
1:B:166:ILE:H	1:B:166:ILE:CD1	2.19	0.52
1:C:139:TYR:CD1	1:C:139:TYR:C	2.83	0.52
1:D:170:LEU:CD2	1:D:177:GLU:HG2	2.40	0.52
1:C:202:LEU:O	1:C:205:TRP:HB3	2.10	0.52
1:C:353:ILE:HD12	1:C:357:SER:HB3	1.91	0.52
1:D:136:ILE:HD11	1:D:201:TYR:CZ	2.45	0.52
1:A:858:ILE:O	1:A:862:VAL:HG23	2.10	0.52
1:A:68:ALA:O	1:A:72:ILE:HG13	2.09	0.52
1:B:93:LEU:HD23	1:B:352:LYS:O	2.10	0.52
1:D:725:LEU:HG	1:D:746:LYS:HZ2	1.75	0.52
1:D:874:LYS:HG3	1:D:875:THR:HG23	1.92	0.52
1:B:818:ASN:O	1:B:819:ILE:C	2.48	0.52
1:C:53:TYR:CE1	1:C:428:GLU:HA	2.45	0.52
1:B:474:GLU:OE2	1:B:477:LYS:HD2	2.10	0.52
1:C:241:ARG:HA	1:C:246:ARG:HD3	1.91	0.52
1:A:301:GLY:O	1:A:330:ARG:NE	2.33	0.52
1:B:594:LEU:HG	1:B:594:LEU:O	2.10	0.52
1:B:625:ILE:HG13	1:B:625:ILE:O	2.10	0.52
1:C:534:SER:O	1:C:538:LEU:HG	2.09	0.52
1:C:793:VAL:HG12	1:C:793:VAL:O	2.10	0.52
1:D:113:PHE:HB2	1:D:137:THR:O	2.10	0.52
1:B:808:ILE:HG22	1:B:812:ASN:ND2	2.20	0.52
1:C:214:THR:HB	1:C:271:LEU:O	2.10	0.52
1:B:422:GLN:HG3	1:B:678:GLN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:VAL:C	1:D:575:PHE:H	2.13	0.52
1:A:135:ALA:HA	1:A:149:PHE:O	2.08	0.52
1:C:169:LYS:O	1:C:175:GLY:HA3	2.09	0.52
1:D:619:TYR:OH	1:D:706:LYS:HG3	2.10	0.52
1:A:529:LYS:HZ3	1:A:529:LYS:HB3	1.75	0.52
1:D:644:THR:O	1:D:648:VAL:HG23	2.09	0.52
1:B:878:LYS:C	1:B:878:LYS:HD3	2.31	0.52
1:A:104:ASP:O	1:A:106:THR:N	2.43	0.52
1:A:806:ARG:HD3	1:A:843:ASP:OD2	2.09	0.52
3:J:105:DC:H2'	3:J:106:DT:C6	2.44	0.51
1:D:813:ARG:O	1:D:815:ILE:N	2.38	0.51
1:C:170:LEU:HA	1:C:177:GLU:CG	2.40	0.51
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.44	0.51
1:C:752:MET:HG2	1:C:889:LEU:CD1	2.40	0.51
1:B:51:ASP:OD1	1:B:53:TYR:N	2.43	0.51
1:C:878:LYS:HB3	1:C:879:PRO:CD	2.40	0.51
1:B:96:THR:HG22	1:B:97:TYR:CE2	2.45	0.51
1:A:740:ALA:HB2	1:A:778:SER:HB2	1.90	0.51
1:D:180:SER:C	1:D:182:ILE:H	2.12	0.51
1:A:897:LEU:N	1:A:897:LEU:HD12	2.18	0.51
1:D:293:ILE:C	1:D:293:ILE:HD12	2.30	0.51
1:B:728:MET:HG3	3:H:113:DC:C5'	2.39	0.51
1:D:52:ILE:HG23	1:D:381:PRO:HD3	1.92	0.51
1:D:87:ASP:OD1	1:D:89:LYS:HG2	2.11	0.51
1:A:901:PHE:O	1:A:902:ASP:HB2	2.09	0.51
1:A:898:PHE:HD1	1:A:898:PHE:H	1.56	0.51
1:C:146:PHE:N	1:C:146:PHE:CD1	2.78	0.51
1:D:17:GLU:HG2	1:D:18:ARG:N	2.24	0.51
1:A:829:LYS:O	1:A:830:VAL:HG13	2.10	0.51
1:C:482:ARG:HH12	1:C:556:GLN:NE2	2.03	0.51
1:C:482:ARG:HB2	1:C:559:ARG:HB3	1.93	0.51
1:A:880:LEU:HD22	1:A:884:THR:HG23	1.92	0.51
1:D:171:GLN:HE22	1:D:303:LEU:HD13	1.75	0.51
1:D:508:LEU:HD23	1:D:534:SER:HB2	1.92	0.51
1:A:153:ASN:HB3	1:A:158:ASN:ND2	2.25	0.51
2:G:16:DG:C2'	2:G:17:DC:H5"	2.40	0.51
1:B:116:GLU:HB3	1:B:135:ALA:HB3	1.93	0.51
1:B:253:ILE:HD12	1:B:254:GLU:N	2.25	0.51
1:C:347:MET:CE	1:C:562:LEU:HD13	2.41	0.51
1:D:263:ILE:N	1:D:263:ILE:HD12	2.26	0.51
1:D:813:ARG:HG3	1:D:814:ALA:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:CG1	1:A:572:ASN:ND2	2.71	0.51
1:A:499:ILE:HD13	1:A:541:MET:HG2	1.92	0.51
1:C:308:PRO:CG	1:C:311:LYS:HG2	2.41	0.51
1:D:178:VAL:HG22	1:D:326:ILE:HD11	1.92	0.51
1:D:434:PHE:CZ	1:D:460:GLY:HA2	2.46	0.51
1:A:767:PHE:CD1	1:A:767:PHE:O	2.64	0.51
1:A:126:PRO:HA	1:A:225:TYR:HD1	1.75	0.51
1:D:645:ASN:OD1	1:D:719:ARG:NH1	2.44	0.51
1:C:592:MET:O	1:C:593:ALA:C	2.49	0.51
1:B:525:GLU:O	1:B:526:ILE:HG23	2.11	0.51
1:C:392:PRO:CG	1:C:584:THR:HG23	2.41	0.51
1:C:514:LEU:HB3	1:C:541:MET:CE	2.41	0.51
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.11	0.51
1:A:685:ARG:NH2	1:A:717:GLY:N	2.59	0.51
1:D:755:GLU:HB3	1:D:759:SER:OG	2.09	0.51
1:B:194:GLU:OE1	1:B:229:ARG:NH2	2.43	0.51
1:B:142:ILE:HG22	1:B:143:ASP:N	2.24	0.51
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.45	0.51
1:B:188:TYR:CE2	1:B:190:PRO:HB3	2.45	0.51
1:A:599:ARG:O	1:A:603:GLU:HG3	2.10	0.51
1:A:836:ARG:NH1	1:A:864:HIS:O	2.44	0.51
1:B:216:TRP:CZ2	1:B:293:ILE:HG21	2.46	0.51
3:L:103:DG:H2"	3:L:104:DG:OP2	2.11	0.51
1:D:458:PRO:HG3	1:D:674:MET:HE1	1.93	0.51
1:D:280:PHE:HB2	1:D:340:PHE:CZ	2.46	0.51
1:D:280:PHE:CE1	1:D:561:LEU:HD11	2.46	0.51
1:B:186:ILE:CG2	1:B:187:ILE:N	2.74	0.51
1:A:506:PRO:HB2	1:A:535:ALA:HA	1.93	0.51
1:C:298:LEU:O	1:C:299:ASN:HB2	2.10	0.51
1:B:863:LEU:HA	1:B:866:MET:CE	2.41	0.51
1:D:516:VAL:HG12	1:D:517:ASP:H	1.75	0.51
1:C:152:LEU:HD22	1:C:160:GLU:HA	1.93	0.51
2:G:8:DT:H2"	2:G:9:DG:C8	2.45	0.51
1:A:255:ASN:ND2	1:A:257:TYR:CD2	2.79	0.51
1:D:197:LEU:C	1:D:197:LEU:HD13	2.31	0.51
1:B:502:ALA:HB1	1:B:535:ALA:HB1	1.93	0.51
1:C:516:VAL:HG21	1:C:522:PHE:CE1	2.45	0.51
1:B:898:PHE:HA	1:B:901:PHE:HD1	1.75	0.51
1:B:376:GLN:NE2	1:B:378:LYS:HZ3	2.09	0.51
1:C:858:ILE:O	1:C:861:ASP:HB2	2.10	0.51
1:D:50:PHE:HA	1:D:55:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:SER:HB3	1:C:166:ILE:HB	1.92	0.50
1:D:458:PRO:C	1:D:460:GLY:H	2.15	0.50
1:A:588:THR:O	1:A:591:GLN:HB2	2.11	0.50
1:A:365:TRP:O	1:A:366:ASP:C	2.50	0.50
1:B:834:PRO:HD2	1:B:871:LEU:HD13	1.92	0.50
1:D:726:LYS:HG3	1:D:726:LYS:O	2.10	0.50
1:D:275:ASP:O	1:D:279:LYS:HB2	2.11	0.50
1:D:305:TYR:CZ	1:D:312:LEU:HD22	2.47	0.50
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.11	0.50
1:D:150:ASP:OD1	1:D:321:ILE:HG12	2.11	0.50
1:C:38:PHE:HB2	1:C:83:LEU:HB2	1.92	0.50
1:C:109:ARG:HD2	1:C:209:THR:O	2.11	0.50
1:C:144:ASP:O	1:C:185:LYS:HD3	2.11	0.50
1:A:514:LEU:HD13	1:A:529:LYS:NZ	2.27	0.50
1:C:506:PRO:CB	1:C:535:ALA:HB2	2.41	0.50
1:B:597:ILE:HD12	1:B:683:MET:SD	2.50	0.50
1:B:445:ALA:HB2	1:B:596:TRP:CH2	2.46	0.50
1:C:436:VAL:HG13	1:C:436:VAL:O	2.11	0.50
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.25	0.50
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.26	0.50
1:C:142:ILE:HA	4:C:915:HOH:O	2.11	0.50
1:B:319:ARG:NH1	1:B:319:ARG:HG2	2.25	0.50
1:A:277:TYR:CE2	1:A:293:ILE:HD12	2.46	0.50
1:C:475:ILE:HD13	1:C:566:LEU:HD22	1.92	0.50
1:A:509:SER:CA	1:A:534:SER:HB3	2.41	0.50
1:D:388:VAL:O	1:D:390:PRO:HD3	2.11	0.50
1:A:759:SER:O	1:A:760:LEU:C	2.48	0.50
1:B:668:ARG:NH1	1:B:668:ARG:CG	2.71	0.50
1:B:162:TRP:HE1	1:B:322:SER:HG	1.57	0.50
1:C:302:LYS:HD3	1:C:303:LEU:H	1.75	0.50
1:C:326:ILE:O	1:C:327:ALA:C	2.49	0.50
1:C:273:TYR:HA	1:C:276:LEU:HB2	1.94	0.50
1:B:708:TYR:CE1	1:B:728:MET:HB3	2.47	0.50
1:D:519:ARG:NH1	1:D:519:ARG:HG3	2.24	0.50
1:B:415:LEU:O	1:B:419:ILE:HG13	2.10	0.50
1:A:197:LEU:HD23	1:A:198:LEU:N	2.27	0.50
1:A:689:ALA:HB1	1:A:711:ASN:O	2.11	0.50
1:B:260:ARG:NH1	1:B:260:ARG:HG2	2.26	0.50
1:A:840:PRO:C	1:A:842:GLY:N	2.65	0.50
1:A:362:ILE:CG1	1:A:572:ASN:HD22	2.24	0.50
1:D:164:ILE:N	1:D:164:ILE:HD13	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:ASN:HA	1:D:857:LEU:CD1	2.42	0.50
1:D:741:VAL:O	1:D:744:ALA:N	2.45	0.50
1:D:82:ALA:H	1:D:382:GLN:NE2	2.09	0.50
1:C:333:GLN:O	1:C:336:ALA:HB3	2.11	0.50
1:D:300:VAL:CG1	1:D:301:GLY:N	2.74	0.50
1:B:728:MET:CG	3:H:113:DC:H5'	2.39	0.50
1:D:576:ARG:HG3	1:D:576:ARG:O	2.11	0.50
1:D:403:ARG:HH22	1:D:889:LEU:CD2	2.24	0.50
1:A:17:GLU:OE2	1:A:29:ARG:NH1	2.44	0.50
1:D:550:VAL:HA	1:D:553:MET:HB3	1.94	0.50
1:C:114:ASP:HB3	1:C:328:VAL:CG2	2.42	0.50
1:A:23:ASN:HD22	1:A:25:ARG:HH22	1.58	0.50
1:A:310:SER:C	1:A:311:LYS:HD3	2.32	0.50
1:B:483:LYS:CB	1:B:483:LYS:NZ	2.75	0.50
1:B:389:GLN:CD	1:B:390:PRO:HD2	2.32	0.50
1:C:642:ARG:CZ	1:C:646:HIS:HB3	2.41	0.50
1:D:846:ILE:HD11	1:D:862:VAL:CG1	2.39	0.50
1:C:109:ARG:HH12	1:C:208:LYS:HD2	1.73	0.50
1:C:449:ARG:NH1	1:C:452:ASP:HA	2.26	0.50
1:A:659:MET:O	1:A:660:GLU:C	2.50	0.50
2:G:6:DA:H2"	2:G:7:DA:H5"	1.94	0.50
1:D:825:VAL:HG12	1:D:826:GLU:N	2.26	0.50
1:A:693:LEU:HD12	1:A:694:GLY:H	1.77	0.50
1:B:786:ASN:O	1:B:787:ASN:HB2	2.12	0.50
1:D:109:ARG:HD3	1:D:209:THR:O	2.11	0.50
1:D:839:ASN:ND2	1:D:839:ASN:N	2.59	0.50
1:B:775:ASN:HB3	1:B:778:SER:OG	2.11	0.50
1:B:488:TYR:C	1:B:490:LEU:H	2.16	0.50
1:A:803:PHE:O	1:A:845:CYS:SG	2.68	0.50
1:D:770:GLU:HG2	1:D:770:GLU:O	2.11	0.50
1:C:738:PRO:HG2	1:C:741:VAL:HG21	1.94	0.50
1:A:145:ARG:HB2	1:A:147:TYR:HE1	1.76	0.50
1:B:687:ALA:HB2	1:B:715:MET:CE	2.40	0.50
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.47	0.50
1:A:219:GLU:O	1:A:219:GLU:HG2	2.12	0.50
3:H:112:DT:H73	4:H:47:HOH:O	2.12	0.50
1:D:502:ALA:HB3	1:D:538:LEU:HD21	1.94	0.50
1:D:493:GLN:HB2	1:D:549:GLU:OE2	2.11	0.50
1:D:131:HIS:HB3	1:D:132:PRO:HD2	1.93	0.50
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.47	0.50
1:D:191:PHE:CB	1:D:197:LEU:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.34	0.49
1:D:321:ILE:HD12	1:D:321:ILE:N	2.27	0.49
1:A:730:LEU:HD22	1:A:883:PHE:CE1	2.46	0.49
1:C:338:ARG:O	1:C:339:GLN:HB2	2.11	0.49
1:C:231:LYS:HE2	1:C:232:ASN:N	2.27	0.49
1:D:835:LEU:HD21	1:D:846:ILE:HG23	1.93	0.49
1:A:555:ALA:HB1	1:A:559:ARG:NH1	2.27	0.49
1:A:422:GLN:O	1:A:676:ASN:HB3	2.12	0.49
1:D:458:PRO:HG3	1:D:674:MET:CE	2.42	0.49
1:C:461:MET:CE	1:C:581:ARG:HD2	2.42	0.49
1:B:887:ALA:O	1:B:888:LYS:HB2	2.12	0.49
1:D:412:LEU:HD21	1:D:683:MET:CE	2.42	0.49
1:B:129:ALA:HB1	1:B:229:ARG:CG	2.42	0.49
1:D:420:ILE:O	1:D:424:ASN:N	2.44	0.49
1:B:245:HIS:CD2	1:B:267:GLY:HA3	2.47	0.49
1:B:247:LYS:HE3	1:B:266:PHE:CE2	2.47	0.49
1:C:138:HIS:CD2	1:C:138:HIS:C	2.85	0.49
1:C:109:ARG:HE	1:C:142:ILE:HD12	1.78	0.49
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.44	0.49
1:C:191:PHE:CE2	1:C:197:LEU:HA	2.48	0.49
1:C:66:ARG:O	1:C:66:ARG:HD2	2.12	0.49
1:B:739:LYS:HE2	1:B:742:GLN:NE2	2.26	0.49
1:A:420:ILE:HG12	1:A:586:ILE:CD1	2.42	0.49
1:D:164:ILE:O	1:D:168:ALA:N	2.40	0.49
1:D:296:PHE:CD1	1:D:297:GLU:N	2.80	0.49
1:A:410:PHE:HB2	1:A:683:MET:HE1	1.93	0.49
1:A:803:PHE:CZ	1:A:845:CYS:HB3	2.47	0.49
1:D:405:LYS:O	1:D:691:PRO:HD3	2.13	0.49
1:B:748:CYS:O	1:B:752:MET:HG3	2.12	0.49
1:A:509:SER:HB3	1:A:534:SER:HB3	1.95	0.49
1:B:644:THR:HG21	1:C:77:ASP:OD2	2.12	0.49
1:A:472:PRO:HA	1:A:475:ILE:HG13	1.94	0.49
1:C:458:PRO:CG	1:C:592:MET:SD	3.01	0.49
1:A:94:SER:HB3	1:A:371:ASN:OD1	2.12	0.49
1:A:51:ASP:OD1	1:A:53:TYR:N	2.44	0.49
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.93	0.49
1:D:533:LEU:HD12	1:D:536:LYS:N	2.27	0.49
3:L:111:DT:H2"	3:L:112:DT:C6	2.47	0.49
1:D:180:SER:O	1:D:182:ILE:N	2.45	0.49
1:B:808:ILE:O	1:B:812:ASN:ND2	2.45	0.49
3:H:105:DC:C6	3:H:106:DT:H72	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:CD1	1:A:526:ILE:HG23	2.40	0.49
1:B:374:LYS:C	1:B:376:GLN:H	2.16	0.49
1:A:195:LYS:HE2	1:A:233:ILE:HG23	1.93	0.49
1:B:722:GLU:HA	1:B:722:GLU:OE1	2.12	0.49
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.42	0.49
1:D:223:ILE:HB	1:D:224:PRO:CD	2.40	0.49
1:A:782:VAL:CG1	1:A:783:SER:N	2.75	0.49
3:L:110:DA:H1'	3:L:111:DT:H5"	1.93	0.49
1:B:273:TYR:CZ	1:B:340:PHE:HB2	2.48	0.49
1:C:83:LEU:N	1:C:83:LEU:HD22	2.28	0.49
1:D:289:SER:O	1:D:293:ILE:HG13	2.13	0.49
2:G:4:CTG:H2'	2:G:5:DG:C8	2.47	0.49
1:A:511:ASP:OD2	1:A:512:GLU:N	2.45	0.49
1:B:773:GLN:H	1:B:773:GLN:NE2	2.10	0.49
1:A:747:GLU:OE2	1:A:747:GLU:HA	2.13	0.49
1:D:795:GLY:HA3	1:D:813:ARG:HD3	1.94	0.49
1:D:180:SER:HA	1:D:183:ILE:HG13	1.95	0.49
1:D:162:TRP:CZ3	1:D:188:TYR:HB2	2.48	0.49
1:B:876:PHE:O	1:B:879:PRO:HG2	2.11	0.49
1:C:110:VAL:HB	1:C:141:SER:HB3	1.94	0.49
1:B:217:ASN:N	1:B:274:ILE:HG21	2.16	0.49
1:B:278:LYS:HE2	1:B:288:TYR:CD2	2.47	0.49
1:D:157:GLY:O	1:D:313:ARG:NH1	2.46	0.49
1:B:858:ILE:HB	1:B:862:VAL:HG23	1.94	0.49
1:D:491:ALA:O	1:D:495:ASN:HB2	2.13	0.49
1:B:233:ILE:HG22	1:B:233:ILE:O	2.12	0.49
1:D:41:CYS:HB3	1:D:57:CYS:CA	2.40	0.49
1:B:362:ILE:HG12	2:G:3:DT:C5'	2.43	0.49
1:A:730:LEU:HB3	1:A:883:PHE:HZ	1.75	0.49
1:C:726:LYS:HG3	1:C:728:MET:CE	2.42	0.49
1:D:668:ARG:HG2	1:D:679:HIS:ND1	2.28	0.49
1:C:171:GLN:C	1:C:173:GLN:H	2.16	0.49
1:B:530:ILE:HG13	1:B:531:LYS:N	2.28	0.49
1:C:495:ASN:HB3	1:C:522:PHE:CD2	2.48	0.49
1:D:419:ILE:HG23	1:D:589:PHE:CD1	2.48	0.49
1:B:398:GLU:OE2	1:B:705:LYS:HE3	2.13	0.49
1:D:514:LEU:CD1	1:D:541:MET:HE1	2.43	0.48
1:D:810:THR:O	1:D:841:PHE:HE1	1.95	0.48
1:C:324:ASN:O	1:C:328:VAL:HG23	2.13	0.48
1:B:270:VAL:HG13	1:B:270:VAL:O	2.12	0.48
1:B:139:TYR:CG	1:B:140:ASP:N	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:PRO:HD3	1:C:699:GLY:HA3	1.94	0.48
1:A:97:TYR:O	1:A:352:LYS:HE3	2.13	0.48
1:C:182:ILE:HD13	1:C:329:TYR:CG	2.48	0.48
1:B:130:LYS:NZ	1:B:130:LYS:HB2	2.28	0.48
3:L:104:DG:C2'	3:L:105:DC:H5"	2.39	0.48
1:C:482:ARG:CZ	1:C:560:LYS:HB2	2.43	0.48
1:A:4:PHE:HD1	1:A:4:PHE:N	2.11	0.48
1:D:582:ASN:O	1:D:585:ALA:HB3	2.12	0.48
1:B:273:TYR:HA	1:B:276:LEU:HD12	1.95	0.48
1:A:380:ILE:HD12	1:A:576:ARG:NE	2.27	0.48
1:D:506:PRO:O	1:D:507:ASN:ND2	2.44	0.48
1:C:203:ASN:HA	1:C:206:GLN:HG2	1.94	0.48
1:C:831:TYR:CE2	1:C:851:GLY:N	2.80	0.48
1:D:559:ARG:O	1:D:562:LEU:HB3	2.14	0.48
1:A:702:TRP:NE1	1:A:708:TYR:HD1	2.11	0.48
1:B:775:ASN:ND2	1:B:777:ILE:H	2.12	0.48
1:A:303:LEU:HB2	1:A:323:TYR:HD1	1.78	0.48
1:B:313:ARG:HG2	1:B:314:GLU:OE1	2.12	0.48
1:A:296:PHE:HD2	1:A:297:GLU:CG	2.26	0.48
1:A:6:LEU:CD1	1:A:26:GLU:HG3	2.43	0.48
1:D:2:LYS:HG2	1:D:3:GLU:H	1.78	0.48
1:D:144:ASP:OD1	1:D:185:LYS:HE3	2.14	0.48
1:B:110:VAL:H	1:B:141:SER:HB3	1.79	0.48
1:D:36:SER:HB3	1:D:59:ARG:NH1	2.28	0.48
1:D:273:TYR:HA	1:D:276:LEU:HD12	1.95	0.48
1:B:499:ILE:HG21	1:B:530:ILE:HD12	1.95	0.48
1:C:204:PHE:O	1:C:208:LYS:HB2	2.14	0.48
1:B:362:ILE:HG12	2:G:3:DT:H5'	1.94	0.48
1:D:360:SER:HB2	1:D:363:LYS:HB3	1.95	0.48
1:B:771:PHE:HD1	1:B:774:LEU:HD12	1.79	0.48
2:G:8:DT:H2'	2:G:9:DG:C8	2.48	0.48
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.95	0.48
1:A:506:PRO:HB2	1:A:535:ALA:CB	2.43	0.48
1:C:426:SER:OG	1:C:427:PRO:HD2	2.14	0.48
1:B:268:ILE:HG22	1:B:269:SER:N	2.29	0.48
1:A:870:VAL:O	1:A:874:LYS:HG2	2.14	0.48
1:D:848:TRP:CB	1:D:854:ILE:HB	2.44	0.48
1:A:126:PRO:HA	1:A:225:TYR:CD1	2.49	0.48
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.95	0.48
3:F:105:DC:H2"	3:F:106:DT:O5'	2.14	0.48
1:A:836:ARG:HH12	1:A:865:TRP:HA	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:SER:CB	1:B:124:PRO:HG3	2.44	0.48
1:C:148:VAL:C	1:C:149:PHE:CD1	2.87	0.48
1:B:324:ASN:O	1:B:327:ALA:HB3	2.14	0.48
1:B:52:ILE:HD12	1:B:428:GLU:HB3	1.94	0.48
1:C:499:ILE:HG21	1:C:542:LEU:HB2	1.94	0.48
1:D:402:ASN:CG	1:D:403:ARG:N	2.66	0.48
1:A:63:ALA:HB3	1:A:67:ASP:OD1	2.14	0.48
1:D:835:LEU:HD13	1:D:839:ASN:OD1	2.14	0.48
1:B:835:LEU:HA	1:B:866:MET:HA	1.95	0.48
1:A:482:ARG:HE	1:A:556:GLN:HE21	1.61	0.48
1:C:109:ARG:HH11	1:C:208:LYS:HA	1.78	0.48
1:D:805:ILE:O	1:D:809:LEU:HG	2.14	0.48
1:C:176:ASP:O	1:C:177:GLU:CB	2.60	0.48
1:B:486:LYS:HB3	1:B:556:GLN:NE2	2.28	0.48
1:B:428:GLU:N	1:B:428:GLU:OE2	2.39	0.48
1:B:796:PHE:HD1	1:B:813:ARG:NH1	2.10	0.48
1:B:772:ARG:CZ	1:B:868:TYR:HB2	2.44	0.48
1:A:195:LYS:HE2	1:A:233:ILE:CG2	2.44	0.48
1:A:737:THR:O	1:A:738:PRO:O	2.31	0.48
3:J:105:DC:H2'	3:J:106:DT:C5	2.48	0.48
1:B:894:LYS:CB	1:B:894:LYS:NZ	2.67	0.48
1:C:85:MET:CA	1:C:380:ILE:HD11	2.42	0.48
1:C:319:ARG:O	1:C:322:SER:N	2.46	0.48
1:B:312:LEU:HD12	1:B:320:TYR:HD1	1.78	0.48
1:D:437:ALA:HB3	1:D:442:TYR:CZ	2.49	0.48
1:B:837:GLU:CG	1:B:838:GLY:N	2.76	0.48
1:B:713:TRP:CZ3	1:B:723:PRO:HD3	2.48	0.48
1:D:136:ILE:HD11	1:D:201:TYR:CE1	2.49	0.48
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.96	0.48
1:A:641:PHE:HA	1:A:646:HIS:CD2	2.48	0.48
1:A:830:VAL:HA	1:A:848:TRP:O	2.14	0.48
1:D:368:ILE:HD11	1:D:562:LEU:HD11	1.96	0.48
1:D:159:VAL:CG1	1:D:160:GLU:H	2.20	0.48
1:D:9:GLU:O	1:D:15:ILE:HA	2.14	0.48
1:D:776:TYR:O	1:D:779:ILE:CD1	2.61	0.48
1:A:41:CYS:HB2	1:A:42:PRO:CD	2.43	0.48
1:B:898:PHE:HA	1:B:901:PHE:CD1	2.49	0.48
1:B:51:ASP:OD1	1:B:51:ASP:C	2.51	0.48
1:A:19:TYR:CE1	1:A:29:ARG:HG2	2.49	0.48
1:B:142:ILE:N	1:B:142:ILE:HD12	2.29	0.48
1:D:727:ILE:HG23	1:D:730:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:LEU:HD11	1:C:558:ASN:ND2	2.29	0.48
1:A:846:ILE:HG13	1:A:846:ILE:O	2.14	0.47
1:C:115:ILE:HG13	1:C:116:GLU:N	2.27	0.47
1:A:708:TYR:HD2	1:A:708:TYR:C	2.18	0.47
1:C:109:ARG:NH1	1:C:208:LYS:HD2	2.29	0.47
1:B:901:PHE:HZ	1:D:650:PHE:HZ	1.59	0.47
1:B:901:PHE:CZ	1:D:650:PHE:HZ	2.32	0.47
1:C:87:ASP:OD2	1:C:90:LEU:HD13	2.13	0.47
1:D:815:ILE:CG2	1:D:858:ILE:HD13	2.41	0.47
1:A:280:PHE:CD2	1:A:343:LEU:HD21	2.49	0.47
1:D:218:VAL:HG12	1:D:223:ILE:HG13	1.97	0.47
1:B:841:PHE:HE1	1:B:858:ILE:HG21	1.79	0.47
1:D:410:PHE:HB3	1:D:683:MET:HG2	1.96	0.47
1:D:597:ILE:HG21	1:D:683:MET:CE	2.44	0.47
1:D:420:ILE:HD12	1:D:420:ILE:N	2.29	0.47
1:C:454:TYR:HB3	1:C:463:TYR:O	2.14	0.47
1:D:461:MET:HA	1:D:461:MET:HE3	1.95	0.47
1:B:405:LYS:HA	1:B:698:ILE:O	2.14	0.47
1:B:693:LEU:HA	4:B:938:HOH:O	2.14	0.47
1:A:780:ALA:HA	1:A:833:LEU:CD2	2.44	0.47
1:D:116:GLU:HG2	1:D:324:ASN:OD1	2.14	0.47
1:A:846:ILE:HD12	1:A:847:ALA:N	2.29	0.47
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.96	0.47
1:B:228:ASN:HA	1:B:231:LYS:HE3	1.95	0.47
1:A:606:ASN:HD21	1:A:613:GLY:HA2	1.76	0.47
3:J:112:DT:H2'	3:J:113:DC:C6	2.50	0.47
1:A:868:TYR:O	1:A:871:LEU:N	2.46	0.47
1:B:466:ASP:OD2	1:B:467:ARG:N	2.47	0.47
1:B:900:MET:O	1:D:635:LYS:HE3	2.14	0.47
1:C:55:LYS:HE2	1:C:55:LYS:N	2.29	0.47
1:D:498:ILE:O	1:D:498:ILE:HG22	2.14	0.47
1:D:37:LEU:HD11	1:D:72:ILE:HD11	1.96	0.47
1:A:864:HIS:HD2	1:A:865:TRP:NE1	2.12	0.47
1:D:489:MET:O	1:D:493:GLN:HG2	2.13	0.47
1:A:43:GLU:N	1:A:43:GLU:OE2	2.47	0.47
1:D:833:LEU:HD22	1:D:834:PRO:HD2	1.96	0.47
1:B:109:ARG:HD2	1:B:140:ASP:OD2	2.14	0.47
1:A:24:GLY:HA3	1:A:107:LYS:HE3	1.96	0.47
1:B:491:ALA:O	1:B:495:ASN:N	2.45	0.47
1:C:188:TYR:C	1:C:189:MET:HG3	2.34	0.47
1:D:647:TRP:CZ3	1:D:651:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PHE:CZ	1:D:222:ALA:HB1	2.49	0.47
3:L:105:DC:H2'	3:L:106:DT:H72	1.97	0.47
1:D:330:ARG:HD3	1:D:333:GLN:OE1	2.15	0.47
1:B:309:ILE:HA	1:B:312:LEU:HB2	1.96	0.47
1:A:522:PHE:HB2	1:A:527:LYS:HE3	1.96	0.47
1:B:486:LYS:O	1:B:490:LEU:HB2	2.15	0.47
1:B:145:ARG:HG2	1:B:187:ILE:HD12	1.96	0.47
1:D:578:TYR:CD1	1:D:579:ASP:N	2.82	0.47
1:B:594:LEU:HD11	1:B:625:ILE:CG2	2.45	0.47
1:C:51:ASP:OD2	1:C:51:ASP:C	2.52	0.47
1:D:514:LEU:H	1:D:541:MET:CE	2.27	0.47
1:C:134:ASP:O	1:C:135:ALA:HB2	2.15	0.47
1:D:117:VAL:HG21	1:D:225:TYR:CE1	2.50	0.47
1:B:330:ARG:HA	1:B:333:GLN:OE1	2.14	0.47
1:C:789:ALA:O	1:C:791:TYR:N	2.48	0.47
1:D:469:GLY:HA3	1:D:472:PRO:HD2	1.96	0.47
1:D:741:VAL:HG13	1:D:876:PHE:HD1	1.80	0.47
1:A:404:TYR:CE1	1:A:618:LEU:HD13	2.50	0.47
1:B:103:TYR:CD1	1:B:103:TYR:N	2.81	0.47
1:B:186:ILE:HG22	1:B:187:ILE:H	1.79	0.47
1:C:118:THR:OG1	1:C:313:ARG:HG3	2.15	0.47
1:D:413:THR:O	1:D:414:SER:C	2.52	0.47
1:B:471:VAL:N	1:B:472:PRO:HD2	2.30	0.47
1:A:602:ASN:HD21	1:A:616:PHE:H	1.62	0.47
1:D:874:LYS:HG3	1:D:875:THR:N	2.29	0.47
1:A:255:ASN:ND2	1:A:257:TYR:HD2	2.12	0.47
1:B:247:LYS:HE3	1:B:266:PHE:CZ	2.50	0.47
1:B:891:TYR:N	1:B:891:TYR:CD2	2.82	0.47
1:D:508:LEU:CD2	1:D:534:SER:HB2	2.45	0.47
1:D:113:PHE:HE1	1:D:218:VAL:HG13	1.79	0.47
3:L:110:DA:C2'	3:L:111:DT:C5'	2.91	0.47
1:B:654:PHE:CE1	1:B:659:MET:HG3	2.50	0.47
1:C:726:LYS:HE2	1:C:728:MET:HE1	1.96	0.47
1:D:825:VAL:HB	1:D:828:GLU:HG2	1.97	0.47
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.80	0.47
1:C:572:ASN:HD21	1:C:574:TRP:HB2	1.80	0.47
1:A:458:PRO:HG3	1:A:592:MET:SD	2.54	0.47
1:A:217:ASN:HA	1:A:272:ASP:OD2	2.14	0.47
1:D:698:ILE:HG12	1:D:752:MET:O	2.15	0.47
1:A:191:PHE:HA	4:A:928:HOH:O	2.15	0.47
3:J:105:DC:C2'	3:J:106:DT:C6	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.44	0.47
1:B:124:PRO:O	1:B:125:GLU:C	2.53	0.47
1:A:21:ASP:OD1	1:A:25:ARG:NH1	2.48	0.47
1:C:659:MET:O	1:C:660:GLU:C	2.53	0.47
1:D:345:LEU:HD23	1:D:355:ILE:HG21	1.95	0.47
1:A:408:MET:HE2	1:A:685:ARG:HD2	1.97	0.47
1:D:777:ILE:HD11	1:D:853:GLU:HA	1.95	0.47
1:A:83:LEU:HD12	1:A:83:LEU:H	1.77	0.47
3:J:110:DA:C2'	3:J:111:DT:H5"	2.45	0.47
1:B:898:PHE:N	1:B:898:PHE:CD1	2.83	0.47
1:B:472:PRO:O	1:B:475:ILE:HG22	2.15	0.47
1:A:105:HIS:ND1	1:A:106:THR:N	2.63	0.47
1:A:786:ASN:N	1:A:786:ASN:HD22	2.12	0.47
1:C:782:VAL:HG12	1:C:783:SER:N	2.30	0.47
1:C:606:ASN:HB3	1:C:611:THR:O	2.15	0.47
1:A:433:THR:HA	1:A:460:GLY:O	2.15	0.47
1:D:892:GLU:O	1:D:894:LYS:HG3	2.15	0.47
1:D:277:TYR:HE1	1:D:338:ARG:CZ	2.28	0.47
1:D:207:GLN:HG2	1:D:208:LYS:HD2	1.96	0.47
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.97	0.47
1:D:793:VAL:CG2	1:D:796:PHE:HB2	2.44	0.47
1:B:800:LYS:O	1:B:800:LYS:HG2	2.14	0.47
1:C:482:ARG:NH1	1:C:556:GLN:HE21	2.06	0.47
1:D:290:LEU:C	1:D:290:LEU:HD23	2.35	0.47
1:B:644:THR:HG23	1:B:645:ASN:H	1.79	0.47
1:D:342:ASN:OD1	1:D:554:THR:HG21	2.15	0.47
1:A:658:ARG:HH11	1:A:658:ARG:HG3	1.79	0.47
1:D:482:ARG:C	1:D:484:GLU:N	2.68	0.46
1:B:516:VAL:HG13	1:B:544:ARG:NH1	2.26	0.46
1:A:606:ASN:ND2	1:A:613:GLY:N	2.60	0.46
3:H:110:DA:H2"	3:H:111:DT:H5"	1.97	0.46
1:D:414:SER:O	1:D:417:PRO:HD2	2.14	0.46
1:C:474:GLU:O	1:C:477:LYS:N	2.44	0.46
1:B:197:LEU:HD23	1:B:197:LEU:O	2.15	0.46
1:D:514:LEU:HD12	1:D:541:MET:HE1	1.98	0.46
1:D:6:LEU:HG	1:D:19:TYR:HA	1.97	0.46
1:A:836:ARG:CD	1:A:866:MET:O	2.64	0.46
1:D:154:SER:HB3	1:D:155:PRO:HD2	1.96	0.46
1:D:345:LEU:O	1:D:349:TYR:HD1	1.98	0.46
1:A:653:LYS:HD3	1:A:657:GLU:OE2	2.15	0.46
2:G:17:DC:H2"	2:G:18:DG:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LEU:CD1	1:D:380:ILE:HG22	2.43	0.46
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.50	0.46
1:A:785:ALA:C	1:A:786:ASN:HD22	2.19	0.46
1:A:406:TYR:CD2	1:A:633:ILE:HG13	2.50	0.46
1:B:731:GLU:HA	1:B:734:LYS:HG2	1.97	0.46
1:B:271:LEU:HB3	1:B:276:LEU:CD1	2.39	0.46
1:B:655:ALA:HA	1:B:659:MET:HB2	1.98	0.46
1:B:790:LYS:HE3	1:B:791:TYR:CZ	2.50	0.46
1:D:764:PHE:CE1	1:D:876:PHE:HE2	2.33	0.46
1:D:280:PHE:HE1	1:D:561:LEU:HD11	1.80	0.46
1:B:197:LEU:HD23	1:B:197:LEU:C	2.36	0.46
1:B:48:LYS:O	1:B:377:ASN:HB3	2.15	0.46
1:A:493:GLN:O	1:A:497:GLU:HG2	2.15	0.46
1:D:95:ASP:O	1:D:97:TYR:N	2.49	0.46
1:D:725:LEU:H	1:D:725:LEU:HD22	1.81	0.46
1:C:671:CYS:SG	1:C:676:ASN:HB2	2.55	0.46
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.36	0.46
1:A:409:SER:O	1:A:686:GLU:HB2	2.14	0.46
1:C:199:MET:O	1:C:202:LEU:HB3	2.16	0.46
1:B:205:TRP:NE1	1:B:242:LEU:O	2.48	0.46
1:D:109:ARG:HH21	1:D:208:LYS:HB3	1.70	0.46
1:B:516:VAL:HG22	1:B:517:ASP:H	1.80	0.46
1:A:741:VAL:C	1:A:743:LYS:N	2.69	0.46
1:A:294:SER:O	1:A:298:LEU:CD1	2.63	0.46
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.51	0.46
1:B:415:LEU:HD11	1:B:419:ILE:HD11	1.98	0.46
1:A:607:GLU:C	1:A:609:CYS:H	2.19	0.46
1:D:218:VAL:HA	1:D:222:ALA:CB	2.41	0.46
1:D:469:GLY:CA	1:D:472:PRO:HD2	2.46	0.46
1:B:231:LYS:HB2	1:B:239:ALA:HB2	1.97	0.46
1:B:533:LEU:HG	1:B:534:SER:H	1.80	0.46
1:C:214:THR:HG21	1:C:341:ILE:CD1	2.45	0.46
1:A:878:LYS:N	1:A:879:PRO:HD2	2.30	0.46
1:B:831:TYR:HD2	1:B:848:TRP:NE1	2.13	0.46
1:A:150:ASP:CG	1:A:317:HIS:HE2	2.18	0.46
1:A:692:PRO:HD2	1:A:695:SER:OG	2.16	0.46
1:C:594:LEU:O	1:C:597:ILE:HG22	2.16	0.46
1:D:202:LEU:HD11	1:D:241:ARG:HB3	1.98	0.46
1:A:362:ILE:HD12	1:A:569:ALA:CB	2.45	0.46
1:C:707:ARG:HB3	1:C:730:LEU:HD23	1.98	0.46
1:D:361:PRO:HB3	1:D:565:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:N	1:B:146:PHE:CD1	2.83	0.46
1:D:218:VAL:CG1	1:D:223:ILE:HG13	2.46	0.46
1:D:230:ILE:HG21	1:D:239:ALA:HA	1.97	0.46
1:C:559:ARG:HA	1:C:559:ARG:HD3	1.78	0.46
1:A:653:LYS:HD2	1:A:653:LYS:C	2.36	0.46
1:C:139:TYR:CD2	1:C:332:LEU:HD21	2.51	0.46
1:C:17:GLU:HG2	1:C:18:ARG:N	2.30	0.46
1:A:36:SER:O	1:A:37:LEU:HD23	2.15	0.46
1:B:505:ASN:HB3	1:B:535:ALA:HB3	1.97	0.46
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.98	0.46
1:D:849:PRO:HG2	1:D:852:THR:HG1	1.80	0.46
1:A:685:ARG:HD2	1:A:688:ILE:HD11	1.97	0.46
2:E:16:DG:H2"	2:E:17:DC:H5"	1.98	0.46
1:A:113:PHE:CE2	1:A:222:ALA:HB1	2.51	0.46
1:A:218:VAL:HG22	1:A:223:ILE:HG13	1.97	0.46
1:A:129:ALA:HB1	1:A:229:ARG:HG2	1.98	0.46
1:B:887:ALA:CB	1:B:889:LEU:HD12	2.46	0.46
1:A:426:SER:OG	1:A:427:PRO:HD2	2.16	0.46
1:D:560:LYS:O	1:D:563:ILE:N	2.49	0.46
1:B:654:PHE:O	1:B:658:ARG:HB2	2.16	0.46
1:C:109:ARG:HH11	1:C:208:LYS:CA	2.29	0.46
1:B:901:PHE:CD2	1:D:608:VAL:HG12	2.51	0.46
1:D:74:ARG:O	1:D:77:ASP:HB2	2.16	0.46
1:A:293:ILE:O	1:A:293:ILE:HG22	2.15	0.46
1:C:17:GLU:OE1	1:C:97:TYR:OH	2.23	0.46
1:A:296:PHE:HD2	1:A:297:GLU:HG2	1.81	0.46
1:B:41:CYS:HB2	1:B:42:PRO:HD2	1.98	0.46
1:C:642:ARG:CD	1:C:642:ARG:N	2.71	0.45
1:A:602:ASN:HD22	1:A:616:PHE:HB2	1.80	0.45
1:A:6:LEU:HD12	1:A:26:GLU:HG3	1.98	0.45
1:A:643:ASP:HA	1:A:693:LEU:HD23	1.97	0.45
1:C:488:TYR:HB3	1:C:519:ARG:HG2	1.98	0.45
1:B:168:ALA:HA	1:B:178:VAL:HG12	1.97	0.45
1:B:61:LEU:CD2	1:B:62:PHE:H	2.29	0.45
1:D:14:SER:HA	1:D:32:GLU:HA	1.98	0.45
1:D:815:ILE:HG22	1:D:858:ILE:CG2	2.30	0.45
1:D:214:THR:HG22	1:D:273:TYR:HB2	1.97	0.45
1:D:182:ILE:C	1:D:182:ILE:HD13	2.36	0.45
1:C:116:GLU:HG3	1:C:324:ASN:HB2	1.98	0.45
1:C:136:ILE:HG22	1:C:137:THR:N	2.31	0.45
1:D:793:VAL:O	1:D:793:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASN:HB3	1:A:404:TYR:CE2	2.50	0.45
1:A:685:ARG:HH11	1:A:688:ILE:HG13	1.79	0.45
1:C:151:LEU:CD2	1:C:154:SER:HB3	2.45	0.45
1:A:213:LEU:HD12	1:A:223:ILE:HD11	1.99	0.45
1:D:576:ARG:HB2	1:D:576:ARG:CZ	2.46	0.45
1:C:454:TYR:HB2	1:C:462:MET:HG2	1.98	0.45
1:C:768:GLU:HG2	1:C:872:LEU:HD21	1.97	0.45
1:B:170:LEU:N	1:B:170:LEU:HD12	2.31	0.45
1:D:187:ILE:O	1:D:187:ILE:HG12	2.15	0.45
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.51	0.45
1:A:835:LEU:HD12	1:A:844:LYS:C	2.36	0.45
1:D:482:ARG:HG2	1:D:559:ARG:CB	2.46	0.45
1:C:130:LYS:O	1:C:229:ARG:NH1	2.49	0.45
1:B:132:PRO:HA	1:B:194:GLU:OE1	2.16	0.45
1:A:42:PRO:O	1:A:45:GLN:N	2.43	0.45
1:A:126:PRO:HG3	1:A:221:PHE:CD1	2.51	0.45
1:D:644:THR:HG21	1:D:713:TRP:CZ2	2.52	0.45
1:B:168:ALA:HA	1:B:178:VAL:CG1	2.46	0.45
1:B:736:SER:HA	1:B:782:VAL:HB	1.98	0.45
1:C:441:ASP:HB3	1:C:447:ALA:HB2	1.98	0.45
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.73	0.45
1:A:87:ASP:OD1	1:A:363:LYS:NZ	2.32	0.45
1:B:123:PHE:CE2	1:B:126:PRO:HD3	2.51	0.45
1:B:231:LYS:CG	1:B:236:GLU:HA	2.39	0.45
2:I:6:DA:H2"	2:I:7:DA:C5'	2.43	0.45
1:C:142:ILE:HG22	1:C:143:ASP:OD1	2.17	0.45
1:A:221:PHE:O	1:A:222:ALA:C	2.54	0.45
1:D:420:ILE:HD11	1:D:586:ILE:HD13	1.98	0.45
1:D:406:TYR:CE2	1:D:691:PRO:HD2	2.51	0.45
1:A:780:ALA:HA	1:A:833:LEU:HD21	1.98	0.45
1:C:572:ASN:ND2	1:C:574:TRP:H	2.15	0.45
1:A:337:LYS:O	1:A:339:GLN:OE1	2.35	0.45
1:A:186:ILE:HG22	1:A:187:ILE:N	2.30	0.45
1:D:180:SER:O	1:D:183:ILE:HG13	2.17	0.45
1:C:132:PRO:HB3	1:C:229:ARG:HH21	1.82	0.45
1:A:680:LEU:HA	1:A:682:PHE:CZ	2.52	0.45
1:B:751:ARG:O	1:B:756:GLY:N	2.33	0.45
1:C:109:ARG:NH1	1:C:208:LYS:CA	2.78	0.45
1:C:145:ARG:HD3	1:C:185:LYS:HB3	1.99	0.45
1:C:274:ILE:CG2	1:C:275:ASP:N	2.78	0.45
1:C:465:LYS:HZ3	1:C:675:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:LYS:NZ	1:D:706:LYS:HB2	2.31	0.45
1:D:250:VAL:HG22	1:D:263:ILE:HG13	1.98	0.45
1:C:458:PRO:HG3	1:C:592:MET:SD	2.57	0.45
1:B:445:ALA:HA	1:B:673:TYR:CE2	2.51	0.45
1:B:389:GLN:OE1	1:B:390:PRO:HD2	2.16	0.45
1:A:112:ASN:ND2	1:A:214:THR:HG23	2.31	0.45
1:B:355:ILE:O	1:B:358:VAL:HG13	2.16	0.45
1:D:422:GLN:OE1	1:D:681:MET:HG2	2.17	0.45
1:D:443:ILE:O	1:D:443:ILE:HG22	2.17	0.45
1:D:132:PRO:N	1:D:229:ARG:HH21	2.14	0.45
1:D:162:TRP:HZ3	1:D:188:TYR:HB2	1.81	0.45
1:D:62:PHE:CD2	1:D:68:ALA:HA	2.51	0.45
1:B:362:ILE:HD11	1:B:572:ASN:CB	2.47	0.45
1:C:351:ALA:O	1:C:352:LYS:HB2	2.17	0.45
1:D:401:PRO:O	1:D:402:ASN:HB2	2.16	0.45
1:C:251:LYS:N	1:C:262:ILE:O	2.50	0.45
1:B:867:ASP:OD1	1:B:870:VAL:HB	2.17	0.45
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.47	0.45
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.99	0.45
1:A:819:ILE:O	1:A:819:ILE:HG13	2.17	0.45
1:A:731:GLU:OE1	1:A:731:GLU:N	2.48	0.45
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.99	0.45
1:A:559:ARG:NH1	1:A:559:ARG:CG	2.74	0.45
1:C:197:LEU:C	1:C:197:LEU:HD23	2.37	0.45
1:C:811:TYR:O	1:C:815:ILE:HG12	2.17	0.45
1:C:223:ILE:CB	1:C:224:PRO:HD3	2.46	0.45
1:C:112:ASN:HA	1:C:214:THR:O	2.17	0.45
1:D:777:ILE:CG2	1:D:831:TYR:HE1	2.30	0.45
1:A:467:ARG:HH11	1:A:467:ARG:CG	2.28	0.45
1:D:216:TRP:CB	1:D:290:LEU:HD12	2.46	0.45
1:D:296:PHE:HD1	1:D:297:GLU:N	2.15	0.45
1:A:412:LEU:HG	1:A:683:MET:HG2	1.98	0.45
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.51	0.45
1:B:597:ILE:O	1:B:601:VAL:HG23	2.17	0.45
1:D:353:ILE:HG13	1:D:354:GLN:O	2.17	0.45
3:F:109:DC:H2"	3:F:110:DA:H5'	1.98	0.45
1:B:218:VAL:HG13	1:B:223:ILE:HG13	1.99	0.45
1:D:663:ILE:O	1:D:664:ASP:C	2.54	0.45
2:G:11:DC:H2"	2:G:12:DA:C5'	2.45	0.45
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.98	0.45
1:D:605:LEU:CD2	1:D:632:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:GLU:HB3	1:D:715:MET:CE	2.47	0.45
1:B:413:THR:O	1:B:414:SER:C	2.55	0.45
1:D:486:LYS:O	1:D:490:LEU:HB2	2.17	0.45
1:D:513:PRO:HA	1:D:541:MET:HE1	1.99	0.45
1:A:503:LEU:CD1	1:A:538:LEU:HB3	2.46	0.45
1:D:835:LEU:HD23	1:D:846:ILE:HG23	1.99	0.45
1:B:530:ILE:HG13	1:B:531:LYS:H	1.82	0.45
1:D:482:ARG:O	1:D:484:GLU:N	2.50	0.45
2:I:6:DA:H1'	2:I:7:DA:H5"	1.99	0.45
1:C:376:GLN:HB2	1:C:378:LYS:HG3	1.99	0.45
1:C:189:MET:O	1:C:191:PHE:HE1	1.99	0.45
1:B:685:ARG:NH2	1:B:714:ASP:OD1	2.50	0.45
1:D:658:ARG:HG3	1:D:658:ARG:NH1	2.30	0.45
1:B:50:PHE:O	1:B:378:LYS:HA	2.17	0.45
1:A:511:ASP:OD1	1:A:533:LEU:HD22	2.16	0.45
1:A:548:THR:O	1:A:551:ALA:N	2.50	0.45
1:B:202:LEU:HD21	1:B:241:ARG:CB	2.47	0.45
1:D:815:ILE:O	1:D:815:ILE:HD12	2.17	0.44
1:B:700:GLY:HA3	1:B:710:LEU:HD23	1.98	0.44
1:A:2:LYS:HE3	3:L:101:DG:O5'	2.17	0.44
1:B:475:ILE:C	1:B:475:ILE:HD13	2.38	0.44
1:D:647:TRP:HZ3	1:D:651:LEU:HD12	1.81	0.44
1:B:810:THR:HG23	1:B:813:ARG:NH2	2.32	0.44
1:B:188:TYR:HE2	1:B:190:PRO:HB3	1.80	0.44
1:C:614:GLU:OE1	1:C:631:LYS:NZ	2.49	0.44
1:B:167:ALA:O	1:B:178:VAL:HG12	2.17	0.44
1:D:535:ALA:HA	1:D:538:LEU:HB2	1.98	0.44
1:D:109:ARG:NH2	1:D:208:LYS:CB	2.76	0.44
1:A:280:PHE:CD2	1:A:343:LEU:CD2	3.00	0.44
1:A:835:LEU:HD12	1:A:844:LYS:O	2.16	0.44
1:B:265:LEU:HD12	1:B:265:LEU:N	2.32	0.44
1:B:797:PRO:HG3	1:B:806:ARG:CZ	2.46	0.44
1:C:81:GLU:HB3	4:C:925:HOH:O	2.16	0.44
3:J:110:DA:H2"	3:J:111:DT:H5"	1.99	0.44
1:C:5:TYR:O	1:C:6:LEU:HD23	2.17	0.44
1:B:92:TYR:O	1:B:96:THR:HB	2.17	0.44
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.90	0.44
1:A:691:PRO:HD3	1:A:699:GLY:HA3	1.99	0.44
1:B:403:ARG:HA	1:B:701:PHE:HA	1.98	0.44
1:B:567:TYR:O	1:B:571:GLY:N	2.49	0.44
1:A:423:VAL:HG12	1:A:423:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLN:HB3	1:D:128:GLN:HE21	1.59	0.44
1:B:776:TYR:OH	1:B:853:GLU:HB3	2.18	0.44
1:D:96:THR:HB	1:D:97:TYR:CD1	2.53	0.44
2:G:10:DA:H2"	2:G:11:DC:H5'	1.97	0.44
1:C:465:LYS:HZ2	1:C:675:ASN:ND2	2.15	0.44
1:D:578:TYR:C	1:D:578:TYR:CD1	2.90	0.44
1:A:506:PRO:HB2	1:A:535:ALA:HB2	1.99	0.44
1:A:249:ARG:HB3	1:A:264:THR:HB	2.00	0.44
1:D:728:MET:SD	3:L:113:DC:H5'	2.57	0.44
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.51	0.44
1:B:250:VAL:O	1:B:250:VAL:HG23	2.16	0.44
1:A:152:LEU:O	1:A:158:ASN:HA	2.17	0.44
1:B:126:PRO:HG3	1:B:221:PHE:CD1	2.50	0.44
1:D:597:ILE:CD1	1:D:663:ILE:HG23	2.44	0.44
1:B:329:TYR:O	1:B:330:ARG:C	2.55	0.44
1:D:864:HIS:C	1:D:866:MET:N	2.67	0.44
1:D:475:ILE:O	1:D:479:PHE:HB2	2.16	0.44
1:C:833:LEU:HD13	1:C:866:MET:HE3	1.98	0.44
1:C:255:ASN:HD22	1:C:255:ASN:HA	1.58	0.44
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.53	0.44
1:D:710:LEU:HD12	1:D:726:LYS:HB3	1.99	0.44
1:D:3:GLU:HB3	1:D:99:TYR:OH	2.16	0.44
1:D:359:PHE:O	1:D:361:PRO:HD3	2.18	0.44
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.99	0.44
1:D:660:GLU:CB	1:D:661:PRO:HD3	2.47	0.44
1:A:61:LEU:HD22	1:A:61:LEU:C	2.38	0.44
1:C:819:ILE:HG23	1:C:819:ILE:O	2.17	0.44
1:D:510:VAL:O	1:D:532:LYS:O	2.36	0.44
1:A:280:PHE:N	1:A:280:PHE:HD1	2.14	0.44
1:A:478:VAL:HG13	1:A:559:ARG:HD2	1.98	0.44
1:D:599:ARG:NH2	1:D:600:LYS:HE2	2.33	0.44
1:A:397:LYS:O	1:A:399:PRO:HD3	2.17	0.44
1:A:868:TYR:O	1:A:869:THR:C	2.55	0.44
1:D:406:TYR:HE2	1:D:647:TRP:CZ2	2.36	0.44
1:D:91:ALA:HA	1:D:370:PHE:HE1	1.83	0.44
1:D:252:VAL:O	1:D:252:VAL:HG23	2.18	0.44
3:J:104:DG:H2"	3:J:105:DC:C6	2.52	0.44
1:D:485:HIS:HB3	1:D:556:GLN:HB3	1.99	0.44
1:B:534:SER:CB	1:B:537:SER:HB2	2.48	0.44
1:A:542:LEU:O	1:A:546:GLN:HG3	2.18	0.44
1:C:147:TYR:N	1:C:147:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:O	1:A:526:ILE:HG22	2.18	0.44
1:D:216:TRP:CZ3	1:D:290:LEU:N	2.86	0.44
1:C:97:TYR:O	1:C:99:TYR:N	2.50	0.44
1:A:145:ARG:HB2	1:A:147:TYR:CE1	2.52	0.44
1:B:110:VAL:H	1:B:141:SER:CB	2.31	0.44
1:B:606:ASN:HD21	1:B:613:GLY:N	2.15	0.44
1:A:8:VAL:O	1:A:354:GLN:NE2	2.47	0.44
1:A:138:HIS:C	1:A:138:HIS:CD2	2.90	0.44
1:D:483:LYS:HG2	1:D:483:LYS:O	2.18	0.44
1:B:775:ASN:ND2	1:B:777:ILE:HB	2.27	0.44
1:C:495:ASN:HB3	1:C:522:PHE:CE2	2.52	0.44
1:B:166:ILE:HG22	1:B:175:GLY:HA2	2.00	0.44
1:A:685:ARG:HH21	1:A:717:GLY:N	2.15	0.44
1:A:410:PHE:N	1:A:410:PHE:HD1	2.16	0.44
1:C:124:PRO:HB2	1:C:225:TYR:CE2	2.52	0.44
1:C:878:LYS:HB3	1:C:879:PRO:HD3	2.00	0.44
1:C:347:MET:HE3	1:C:562:LEU:HD13	1.98	0.44
1:D:496:GLY:HA2	1:D:499:ILE:CD1	2.47	0.44
1:D:119:SER:HA	1:D:120:PRO:HD3	1.80	0.44
1:A:846:ILE:HD11	1:A:854:ILE:HD11	2.00	0.44
1:A:804:HIS:NE2	3:F:110:DA:OP1	2.38	0.44
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.53	0.44
1:B:700:GLY:HA2	1:B:753:LEU:CD2	2.44	0.44
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.65	0.44
1:A:402:ASN:HA	1:A:886:ALA:O	2.18	0.44
1:D:96:THR:C	1:D:97:TYR:CD1	2.91	0.44
1:B:475:ILE:HD13	1:B:475:ILE:O	2.18	0.44
1:B:25:ARG:NH1	1:B:25:ARG:HG2	2.31	0.44
1:A:797:PRO:HB3	1:A:806:ARG:HG3	2.00	0.44
1:C:343:LEU:CD1	1:C:558:ASN:ND2	2.81	0.44
1:A:75:MET:HE3	1:A:80:LEU:O	2.18	0.44
1:C:194:GLU:O	1:C:195:LYS:C	2.55	0.43
1:B:115:ILE:HD11	1:B:221:PHE:CD2	2.53	0.43
1:C:840:PRO:HD2	1:C:865:TRP:CD1	2.53	0.43
1:A:811:TYR:OH	1:A:815:ILE:HD13	2.18	0.43
1:A:536:LYS:C	1:A:536:LYS:HD3	2.38	0.43
1:A:514:LEU:HD22	1:A:529:LYS:HE2	1.99	0.43
1:C:761:GLN:HE22	1:C:893:LYS:HA	1.82	0.43
1:C:475:ILE:CG2	1:C:476:THR:N	2.79	0.43
1:C:10:GLN:OE1	1:C:65:MET:HE3	2.18	0.43
1:B:143:ASP:O	1:B:144:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HE3	1:B:576:ARG:HH22	1.83	0.43
1:C:839:ASN:HB2	1:C:840:PRO:HD2	2.00	0.43
1:D:428:GLU:OE1	1:D:469:GLY:HA2	2.18	0.43
1:D:779:ILE:HD13	1:D:780:ALA:N	2.33	0.43
1:C:7:THR:CG2	1:C:211:VAL:HG13	2.48	0.43
1:B:52:ILE:O	1:B:428:GLU:HG3	2.18	0.43
1:B:365:TRP:CE2	1:B:566:LEU:HD13	2.53	0.43
1:B:96:THR:HG22	1:B:96:THR:O	2.18	0.43
1:D:50:PHE:N	1:D:50:PHE:CD1	2.87	0.43
1:C:606:ASN:OD1	1:C:614:GLU:HB2	2.18	0.43
1:A:782:VAL:O	1:A:783:SER:HB2	2.17	0.43
1:A:831:TYR:N	1:A:848:TRP:O	2.51	0.43
1:D:317:HIS:CE1	1:D:321:ILE:HD13	2.53	0.43
1:A:240:LYS:O	1:A:246:ARG:HA	2.18	0.43
1:B:744:ALA:O	1:B:747:GLU:HB3	2.19	0.43
1:D:33:TYR:CE2	1:D:35:PRO:HA	2.52	0.43
1:B:517:ASP:OD1	1:B:519:ARG:CB	2.64	0.43
1:D:326:ILE:HG22	1:D:330:ARG:HE	1.82	0.43
1:B:685:ARG:CG	1:B:685:ARG:HH11	2.32	0.43
1:C:151:LEU:HD11	1:C:153:ASN:O	2.18	0.43
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.99	0.43
1:A:871:LEU:O	1:A:875:THR:OG1	2.34	0.43
1:A:159:VAL:HG21	1:A:317:HIS:CG	2.53	0.43
1:A:702:TRP:NE1	1:A:708:TYR:CD1	2.86	0.43
1:C:661:PRO:O	1:C:662:ALA:C	2.55	0.43
1:A:2:LYS:HA	1:A:2:LYS:CE	2.48	0.43
1:D:771:PHE:CE2	1:D:872:LEU:HB2	2.53	0.43
1:A:869:THR:O	1:A:873:GLU:HB2	2.18	0.43
1:A:741:VAL:HG11	1:A:875:THR:O	2.19	0.43
1:D:285:GLN:HE21	1:D:285:GLN:N	2.15	0.43
1:B:771:PHE:CD1	1:B:774:LEU:HD12	2.52	0.43
1:A:643:ASP:CA	1:A:693:LEU:HD23	2.48	0.43
1:B:150:ASP:HB3	1:B:188:TYR:CE1	2.53	0.43
1:D:709:ALA:HB2	1:D:730:LEU:HD11	1.99	0.43
1:A:431:ALA:N	1:A:462:MET:O	2.44	0.43
1:D:236:GLU:O	1:D:240:LYS:HG2	2.18	0.43
1:D:839:ASN:ND2	1:D:839:ASN:O	2.51	0.43
1:D:212:ILE:CD1	1:D:345:LEU:HD21	2.43	0.43
1:B:233:ILE:CD1	1:B:233:ILE:N	2.82	0.43
1:C:412:LEU:HG	1:C:683:MET:HE3	2.00	0.43
1:C:312:LEU:O	1:C:313:ARG:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HG	1:A:19:TYR:HA	2.01	0.43
1:C:607:GLU:O	1:C:609:CYS:N	2.52	0.43
1:C:898:PHE:N	1:C:898:PHE:CD2	2.85	0.43
1:D:493:GLN:CG	1:D:494:ARG:H	2.14	0.43
1:D:113:PHE:CE1	1:D:218:VAL:HG13	2.54	0.43
1:C:164:ILE:HG13	1:C:183:ILE:HD11	2.01	0.43
1:A:45:GLN:O	1:A:46:ALA:C	2.56	0.43
1:C:271:LEU:HD21	1:C:356:GLN:HA	2.01	0.43
1:B:396:VAL:HB	2:G:7:DA:OP1	2.19	0.43
1:A:745:LEU:CD1	1:A:876:PHE:CD1	3.01	0.43
1:A:5:TYR:HA	1:A:19:TYR:CB	2.49	0.43
1:A:775:ASN:O	1:A:778:SER:N	2.44	0.43
1:A:825:VAL:HG22	1:A:826:GLU:N	2.33	0.43
1:D:253:ILE:HG13	1:D:253:ILE:O	2.18	0.43
1:A:279:LYS:HB3	1:A:280:PHE:CE1	2.54	0.43
1:D:133:ILE:HG12	1:D:229:ARG:CD	2.38	0.43
1:D:491:ALA:HB1	1:D:521:ASP:OD1	2.18	0.43
1:B:330:ARG:O	1:B:334:ILE:HG13	2.19	0.43
2:G:15:DC:H2'	2:G:16:DG:C8	2.53	0.43
1:A:529:LYS:NZ	1:A:529:LYS:HB3	2.34	0.43
1:A:109:ARG:HD2	1:A:209:THR:O	2.19	0.43
1:C:202:LEU:CD2	1:C:241:ARG:HH21	2.31	0.43
1:C:458:PRO:HG2	1:C:592:MET:SD	2.59	0.43
1:A:389:GLN:HB3	1:A:389:GLN:HE21	1.54	0.43
1:D:687:ALA:HA	1:D:714:ASP:O	2.19	0.43
1:D:109:ARG:NH2	1:D:140:ASP:OD2	2.52	0.43
1:A:835:LEU:O	1:A:837:GLU:N	2.52	0.43
3:F:110:DA:C2'	3:F:111:DT:C5'	2.94	0.43
1:C:412:LEU:HG	1:C:683:MET:HE2	1.99	0.43
1:B:446:VAL:O	1:B:446:VAL:CG2	2.60	0.43
1:C:251:LYS:O	1:C:261:GLU:HA	2.19	0.43
1:B:130:LYS:NZ	1:B:130:LYS:CB	2.81	0.43
1:C:496:GLY:O	1:C:500:LYS:HG3	2.18	0.43
1:B:443:ILE:HD13	1:B:595:GLN:HB3	2.00	0.43
1:C:702:TRP:CZ3	1:C:710:LEU:HD21	2.53	0.43
1:B:211:VAL:HG12	1:B:211:VAL:O	2.17	0.43
1:D:19:TYR:CD1	1:D:19:TYR:N	2.86	0.43
1:B:727:ILE:HG23	1:B:730:LEU:HD12	2.01	0.43
1:D:230:ILE:CG2	1:D:239:ALA:HA	2.49	0.43
1:D:132:PRO:CA	1:D:229:ARG:NH2	2.79	0.43
1:C:133:ILE:HG13	1:C:229:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PHE:HZ	1:D:71:TRP:CE3	2.37	0.43
1:A:779:ILE:O	1:A:871:LEU:HD21	2.18	0.43
1:D:417:PRO:O	1:D:420:ILE:N	2.52	0.43
1:C:836:ARG:NH1	1:C:836:ARG:HG3	2.34	0.43
1:B:517:ASP:C	1:B:519:ARG:H	2.22	0.43
1:B:412:LEU:HB2	1:B:623:ASP:HB2	2.01	0.43
1:C:271:LEU:HB3	1:C:276:LEU:HD21	2.00	0.43
1:B:135:ALA:HB1	1:B:324:ASN:HD22	1.84	0.43
1:B:186:ILE:O	1:B:187:ILE:CG1	2.67	0.43
1:C:154:SER:OG	1:C:313:ARG:NH2	2.52	0.43
1:D:73:LYS:O	1:D:77:ASP:OD2	2.36	0.43
1:D:573:VAL:HA	1:D:578:TYR:CD2	2.54	0.43
1:A:120:PRO:HG2	1:A:156:TYR:HE1	1.81	0.43
1:D:825:VAL:HB	1:D:828:GLU:HG3	2.00	0.43
1:B:170:LEU:CD1	1:B:170:LEU:N	2.82	0.43
1:B:880:LEU:O	1:B:884:THR:HG23	2.19	0.43
1:B:441:ASP:HB3	1:B:447:ALA:HB2	2.00	0.43
1:B:555:ALA:O	1:B:559:ARG:HD3	2.18	0.43
1:B:214:THR:OG1	1:B:273:TYR:HD2	2.02	0.42
1:D:803:PHE:O	1:D:806:ARG:HB2	2.19	0.42
1:B:331:VAL:O	1:B:334:ILE:HB	2.19	0.42
1:A:45:GLN:O	1:A:47:THR:HG23	2.18	0.42
1:B:186:ILE:CG2	1:B:187:ILE:H	2.32	0.42
1:B:145:ARG:HG2	1:B:187:ILE:CD1	2.48	0.42
1:D:125:GLU:HG3	1:D:127:SER:HB3	2.00	0.42
1:A:294:SER:O	1:A:298:LEU:HD12	2.19	0.42
1:C:461:MET:SD	1:C:581:ARG:HB3	2.59	0.42
1:A:299:ASN:O	1:A:300:VAL:HB	2.18	0.42
1:A:562:LEU:O	1:A:563:ILE:C	2.56	0.42
1:D:597:ILE:CG2	1:D:598:GLU:N	2.82	0.42
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.34	0.42
1:C:413:THR:O	1:C:414:SER:C	2.57	0.42
1:C:323:TYR:O	1:C:326:ILE:N	2.52	0.42
1:B:685:ARG:CZ	1:B:688:ILE:HD11	2.48	0.42
1:A:656:ARG:HA	1:A:660:GLU:CG	2.48	0.42
1:B:76:GLU:OE1	1:B:382:GLN:NE2	2.52	0.42
1:A:745:LEU:O	1:A:749:ILE:HG13	2.19	0.42
1:A:741:VAL:C	1:A:743:LYS:H	2.22	0.42
1:C:453:VAL:CG2	1:C:454:TYR:N	2.82	0.42
1:B:597:ILE:CD1	1:B:683:MET:SD	3.07	0.42
1:A:502:ALA:O	1:A:503:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ALA:C	1:C:136:ILE:HG13	2.38	0.42
1:C:321:ILE:O	1:C:325:ILE:HG13	2.19	0.42
2:K:7:DA:H2"	2:K:8:DT:OP2	2.20	0.42
1:D:484:GLU:OE1	1:D:485:HIS:ND1	2.43	0.42
2:G:10:DA:C2'	2:G:11:DC:H5"	2.48	0.42
1:A:621:ASP:HB3	3:F:114:DA:C5'	2.50	0.42
2:G:6:DA:C2'	2:G:7:DA:H5"	2.49	0.42
2:E:15:DC:H2"	2:E:16:DG:C8	2.54	0.42
1:A:120:PRO:CG	1:A:156:TYR:CE1	3.02	0.42
1:C:9:GLU:HG3	1:C:267:GLY:H	1.85	0.42
1:D:456:CYS:HB3	1:D:461:MET:O	2.19	0.42
1:B:120:PRO:HG2	1:B:156:TYR:HE2	1.82	0.42
1:C:503:LEU:HG	1:C:538:LEU:HB3	2.01	0.42
1:B:840:PRO:HD3	1:B:865:TRP:CE2	2.55	0.42
1:D:105:HIS:ND1	1:D:106:THR:N	2.67	0.42
1:C:254:GLU:HG2	1:C:259:SER:HB2	2.01	0.42
1:D:241:ARG:C	1:D:243:SER:H	2.23	0.42
2:K:8:DT:C2'	2:K:9:DG:C8	3.03	0.42
1:D:391:TYR:HB2	1:D:392:PRO:CD	2.42	0.42
1:A:397:LYS:HD3	1:A:619:TYR:HA	2.00	0.42
1:C:109:ARG:NH1	1:C:208:LYS:CD	2.79	0.42
1:A:83:LEU:N	1:A:83:LEU:CD1	2.82	0.42
1:B:422:GLN:HG2	1:B:676:ASN:HB3	2.00	0.42
1:C:506:PRO:C	1:C:507:ASN:HD22	2.23	0.42
1:D:870:VAL:O	1:D:874:LYS:HG2	2.19	0.42
1:D:655:ALA:HA	1:D:659:MET:HB2	2.01	0.42
1:D:244:PRO:O	1:D:245:HIS:HD2	2.02	0.42
1:C:264:THR:O	1:C:265:LEU:HD23	2.20	0.42
2:I:3:DT:H5'	2:I:3:DT:C6	2.55	0.42
1:C:128:GLN:HE21	1:C:128:GLN:HB3	1.61	0.42
1:C:722:GLU:HA	1:C:722:GLU:OE1	2.20	0.42
1:D:33:TYR:OH	1:D:95:ASP:OD2	2.31	0.42
1:C:143:ASP:O	1:C:144:ASP:CB	2.67	0.42
1:B:408:MET:HE1	1:B:685:ARG:HD3	2.00	0.42
1:A:408:MET:HE3	1:A:655:ALA:HB2	1.99	0.42
1:C:97:TYR:HA	1:C:99:TYR:CE1	2.54	0.42
1:B:442:TYR:O	1:B:596:TRP:HZ3	2.02	0.42
1:D:616:PHE:O	1:D:627:VAL:HA	2.19	0.42
1:A:206:GLN:OE1	1:A:241:ARG:HB3	2.19	0.42
1:C:635:LYS:HD2	1:C:635:LYS:O	2.19	0.42
1:B:757:GLU:O	1:B:761:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:ALA:HB1	1:D:539:ASN:HD21	1.82	0.42
1:B:273:TYR:O	1:B:277:TYR:HB2	2.20	0.42
1:B:841:PHE:CE2	1:B:862:VAL:HG22	2.54	0.42
1:A:2:LYS:NZ	1:A:2:LYS:CA	2.74	0.42
1:C:28:THR:O	1:C:28:THR:CG2	2.67	0.42
1:A:410:PHE:HA	1:A:684:ASP:O	2.20	0.42
1:B:425:ILE:HG23	1:B:463:TYR:CZ	2.54	0.42
1:B:831:TYR:CD2	1:B:850:SER:HA	2.55	0.42
1:C:570:LEU:HD23	1:C:575:PHE:HE2	1.84	0.42
1:C:249:ARG:O	1:C:263:ILE:HA	2.20	0.42
1:C:249:ARG:HB3	1:C:264:THR:HB	2.02	0.42
1:C:285:GLN:O	1:C:829:LYS:NZ	2.45	0.42
1:D:493:GLN:HB3	1:D:549:GLU:HG3	2.02	0.42
1:A:824:VAL:HG13	1:A:849:PRO:CG	2.47	0.42
1:C:514:LEU:HB3	1:C:541:MET:HE1	2.00	0.42
1:C:147:TYR:CB	1:C:149:PHE:HE1	2.30	0.42
1:D:294:SER:C	1:D:296:PHE:N	2.73	0.42
1:A:140:ASP:OD1	1:A:142:ILE:N	2.53	0.42
1:A:643:ASP:C	1:A:693:LEU:HD23	2.39	0.42
1:A:94:SER:HG	1:A:370:PHE:HE2	1.64	0.42
1:A:50:PHE:CD2	1:A:56:PRO:HA	2.54	0.42
1:B:125:GLU:HA	1:B:126:PRO:HD3	1.90	0.42
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.55	0.42
1:A:384:ARG:HG3	1:A:386:HIS:CE1	2.54	0.42
1:D:101:ILE:O	1:D:102:LYS:HE3	2.20	0.42
1:A:606:ASN:ND2	1:A:613:GLY:HA2	2.35	0.42
1:D:234:PHE:CD1	1:D:234:PHE:N	2.87	0.42
1:B:702:TRP:CZ2	1:B:708:TYR:CD2	3.08	0.42
1:A:277:TYR:HA	1:A:340:PHE:CE2	2.55	0.42
1:A:150:ASP:OD1	1:A:317:HIS:NE2	2.52	0.42
1:B:96:THR:HG22	1:B:97:TYR:CD2	2.55	0.42
1:B:604:TYR:O	1:B:607:GLU:HB3	2.20	0.42
1:A:861:ASP:N	1:A:861:ASP:OD2	2.52	0.42
1:D:526:ILE:HG13	1:D:526:ILE:O	2.19	0.42
1:D:839:ASN:ND2	1:D:839:ASN:H	2.18	0.42
1:D:839:ASN:OD1	1:D:843:ASP:O	2.38	0.42
1:A:736:SER:HB2	1:A:782:VAL:O	2.20	0.42
1:A:171:GLN:HE22	1:A:319:ARG:NH1	2.10	0.42
1:B:151:LEU:HG	1:B:153:ASN:O	2.20	0.42
1:C:482:ARG:NH1	1:C:556:GLN:HG2	2.35	0.42
1:C:149:PHE:N	1:C:149:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:PHE:O	1:C:222:ALA:C	2.58	0.42
1:D:147:TYR:CD1	1:D:147:TYR:N	2.87	0.42
3:H:110:DA:C2'	3:H:111:DT:H5"	2.50	0.42
1:B:678:GLN:HG2	1:B:680:LEU:HG	2.01	0.42
1:A:82:ALA:O	1:A:382:GLN:HB2	2.20	0.42
1:B:472:PRO:HA	1:B:475:ILE:HG22	2.01	0.42
1:B:374:LYS:O	1:B:376:GLN:N	2.52	0.42
1:C:457:SER:HA	1:C:458:PRO:HD3	1.86	0.42
1:A:734:LYS:HB3	1:A:737:THR:OG1	2.20	0.42
1:B:761:GLN:OE1	1:B:893:LYS:HE3	2.19	0.42
1:A:799:PRO:HD2	4:A:920:HOH:O	2.19	0.42
1:C:692:PRO:HD2	1:C:695:SER:OG	2.19	0.42
1:B:499:ILE:HG13	1:B:542:LEU:HD13	2.02	0.42
1:A:621:ASP:HB3	3:F:114:DA:H5"	2.02	0.42
1:B:362:ILE:CD1	1:B:575:PHE:HB2	2.50	0.42
1:B:706:LYS:HE2	3:H:113:DC:O2	2.20	0.42
1:D:771:PHE:CD2	1:D:872:LEU:HD13	2.55	0.42
1:A:159:VAL:HG23	1:A:160:GLU:O	2.20	0.42
1:B:559:ARG:O	1:B:563:ILE:HG13	2.19	0.42
1:C:254:GLU:HG2	1:C:259:SER:CB	2.50	0.42
1:A:415:LEU:O	1:A:419:ILE:HG13	2.20	0.42
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.84	0.42
1:C:292:TYR:O	1:C:295:GLU:HB3	2.19	0.41
1:D:423:VAL:HB	1:D:425:ILE:HG13	2.00	0.41
1:B:312:LEU:HD12	1:B:320:TYR:CD1	2.55	0.41
1:C:524:ASP:HA	1:C:527:LYS:HE3	2.01	0.41
1:B:116:GLU:HA	1:B:116:GLU:OE1	2.19	0.41
3:J:112:DT:H2'	3:J:113:DC:C5	2.55	0.41
1:B:901:PHE:HB3	1:D:608:VAL:CG1	2.50	0.41
1:A:602:ASN:ND2	1:A:616:PHE:H	2.18	0.41
1:A:150:ASP:OD1	1:A:188:TYR:OH	2.33	0.41
1:A:389:GLN:HA	1:A:390:PRO:HD3	1.83	0.41
1:B:13:ASP:OD2	1:B:66:ARG:HB2	2.20	0.41
2:E:6:DA:C2'	2:E:7:DA:C5'	2.84	0.41
1:A:839:ASN:HB3	1:A:865:TRP:CE3	2.55	0.41
1:D:131:HIS:HB2	1:D:225:TYR:OH	2.20	0.41
1:D:358:VAL:HG12	1:D:358:VAL:O	2.20	0.41
1:B:248:THR:CG2	1:B:265:LEU:HA	2.44	0.41
1:A:618:LEU:HG	1:A:619:TYR:N	2.34	0.41
1:B:621:ASP:O	1:B:623:ASP:N	2.51	0.41
1:A:516:VAL:CG1	1:A:526:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD21	1:A:529:LYS:HE2	2.01	0.41
1:A:297:GLU:C	1:A:298:LEU:HD12	2.41	0.41
1:B:463:TYR:CD1	1:B:463:TYR:N	2.88	0.41
1:C:261:GLU:H	1:C:261:GLU:HG2	1.74	0.41
1:D:686:GLU:HA	1:D:686:GLU:OE1	2.20	0.41
1:C:256:MET:HB3	1:C:257:TYR:CD1	2.55	0.41
1:D:129:ALA:HB1	1:D:225:TYR:CE2	2.55	0.41
1:D:478:VAL:HG11	1:D:562:LEU:HD22	2.03	0.41
1:B:132:PRO:HB3	1:B:194:GLU:OE2	2.20	0.41
1:B:235:GLY:O	1:B:236:GLU:C	2.58	0.41
1:A:811:TYR:HH	1:A:822:PRO:C	2.23	0.41
1:C:303:LEU:HB3	1:C:319:ARG:HH11	1.85	0.41
1:C:752:MET:CE	1:C:889:LEU:HD12	2.50	0.41
1:D:699:GLY:C	1:D:753:LEU:HD22	2.40	0.41
1:B:61:LEU:HD23	1:B:62:PHE:H	1.85	0.41
1:D:496:GLY:HA2	1:D:499:ILE:HD12	2.03	0.41
1:A:800:LYS:O	1:A:802:PRO:HD3	2.21	0.41
3:L:108:DT:H2"	3:L:109:DC:O5'	2.21	0.41
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.78	0.41
1:C:32:GLU:HA	1:C:32:GLU:OE1	2.20	0.41
1:A:841:PHE:O	1:A:842:GLY:C	2.58	0.41
1:A:279:LYS:HE2	1:A:359:PHE:HA	2.00	0.41
1:D:218:VAL:HG12	1:D:223:ILE:CD1	2.50	0.41
1:B:193:ASN:HB3	1:B:196:GLU:CG	2.50	0.41
1:C:148:VAL:C	1:C:149:PHE:HD1	2.24	0.41
1:C:811:TYR:CA	1:C:846:ILE:HD11	2.50	0.41
1:D:296:PHE:CD1	1:D:296:PHE:C	2.94	0.41
2:E:16:DG:N2	3:F:103:DG:C2	2.89	0.41
1:A:6:LEU:HD13	1:A:211:VAL:HG21	2.01	0.41
1:A:776:TYR:CE2	1:A:777:ILE:HG13	2.56	0.41
1:A:776:TYR:CG	1:A:863:LEU:HD11	2.55	0.41
1:B:834:PRO:O	1:B:867:ASP:N	2.50	0.41
1:C:558:ASN:HA	1:C:558:ASN:HD22	1.65	0.41
1:D:421:ARG:CD	1:D:475:ILE:HG23	2.51	0.41
1:D:91:ALA:O	1:D:94:SER:HB2	2.19	0.41
1:C:33:TYR:OH	1:C:95:ASP:OD1	2.32	0.41
1:A:809:LEU:HD23	1:A:812:ASN:ND2	2.36	0.41
1:C:520:PHE:O	1:C:521:ASP:C	2.58	0.41
1:D:533:LEU:HB3	1:D:537:SER:OG	2.20	0.41
1:D:18:ARG:HH21	1:D:211:VAL:HG22	1.84	0.41
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ALA:H	1:D:382:GLN:CG	2.33	0.41
1:C:414:SER:O	1:C:415:LEU:C	2.57	0.41
1:C:147:TYR:N	1:C:147:TYR:HD1	2.17	0.41
1:A:725:LEU:HD12	1:A:746:LYS:HE2	2.02	0.41
1:B:209:THR:HA	1:B:210:PRO:HD3	1.80	0.41
1:C:731:GLU:OE2	1:C:879:PRO:HB3	2.20	0.41
1:D:825:VAL:HG12	1:D:826:GLU:H	1.86	0.41
1:A:471:VAL:HB	1:A:472:PRO:HD3	2.01	0.41
1:A:334:ILE:O	1:A:337:LYS:HB2	2.20	0.41
1:B:416:TYR:HB2	1:B:417:PRO:HD3	2.02	0.41
1:B:546:GLN:O	1:B:550:VAL:HG23	2.21	0.41
1:C:561:LEU:HA	1:C:561:LEU:HD12	1.82	0.41
1:C:577:TYR:N	1:C:577:TYR:CD2	2.88	0.41
1:D:890:ASP:N	1:D:890:ASP:OD2	2.51	0.41
1:B:280:PHE:N	1:B:280:PHE:CD1	2.88	0.41
1:B:494:ARG:C	1:B:496:GLY:H	2.23	0.41
1:D:533:LEU:HD11	1:D:536:LYS:HB2	2.03	0.41
2:I:12:DA:H2"	2:I:13:DG:C5'	2.50	0.41
1:B:85:MET:HA	1:B:380:ILE:HD11	2.03	0.41
1:B:727:ILE:HB	1:B:733:GLN:NE2	2.36	0.41
1:D:602:ASN:HD21	1:D:617:VAL:HG22	1.86	0.41
1:D:425:ILE:O	1:D:426:SER:HB2	2.20	0.41
1:C:140:ASP:OD1	1:C:142:ILE:HB	2.21	0.41
1:C:189:MET:O	1:C:191:PHE:CD1	2.74	0.41
2:G:15:DC:H2"	2:G:16:DG:C5'	2.50	0.41
1:A:396:VAL:HG21	1:A:706:LYS:NZ	2.35	0.41
1:A:467:ARG:H	1:A:467:ARG:HD3	1.85	0.41
2:G:5:DG:H2"	2:G:6:DA:O5'	2.21	0.41
1:C:761:GLN:NE2	1:C:893:LYS:HA	2.36	0.41
1:C:97:TYR:N	1:C:97:TYR:CD1	2.89	0.41
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.51	0.41
1:D:416:TYR:HD2	1:D:586:ILE:HG22	1.85	0.41
1:C:420:ILE:HG21	1:C:471:VAL:HG12	2.03	0.41
1:C:493:GLN:HA	1:C:549:GLU:OE2	2.21	0.41
1:B:783:SER:O	1:B:829:LYS:HA	2.20	0.41
1:A:52:ILE:HD12	1:A:428:GLU:HB3	2.03	0.41
1:C:839:ASN:C	1:C:841:PHE:H	2.24	0.41
1:C:516:VAL:HG21	1:C:522:PHE:HE1	1.82	0.41
1:D:470:VAL:HG13	1:D:471:VAL:N	2.36	0.41
1:C:162:TRP:HB3	1:C:188:TYR:CE2	2.55	0.41
1:C:111:ALA:HB2	1:C:210:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:ARG:HD2	1:D:685:ARG:O	2.21	0.41
1:B:837:GLU:HG2	1:B:838:GLY:H	1.82	0.41
1:D:578:TYR:OH	1:D:580:LEU:HD13	2.21	0.41
1:B:810:THR:HG22	1:B:810:THR:O	2.21	0.41
1:C:738:PRO:HG2	1:C:741:VAL:HB	2.02	0.41
1:A:506:PRO:HB2	1:A:535:ALA:CA	2.50	0.41
1:B:104:ASP:C	1:B:104:ASP:OD2	2.58	0.41
1:D:560:LYS:C	1:D:562:LEU:N	2.74	0.41
1:D:321:ILE:CD1	1:D:321:ILE:N	2.83	0.41
1:A:175:GLY:O	1:A:319:ARG:NH2	2.53	0.41
1:A:231:LYS:O	1:A:235:GLY:N	2.44	0.41
1:D:373:LEU:O	1:D:378:LYS:HB2	2.20	0.41
1:D:216:TRP:O	1:D:217:ASN:HB2	2.21	0.41
1:A:660:GLU:HB2	1:A:661:PRO:CD	2.49	0.41
1:C:757:GLU:O	1:C:761:GLN:HG3	2.20	0.41
1:A:194:GLU:CD	1:A:229:ARG:NH1	2.74	0.41
1:D:170:LEU:HD22	1:D:177:GLU:OE2	2.20	0.41
1:A:602:ASN:HD21	1:A:616:PHE:N	2.18	0.41
1:D:2:LYS:CG	1:D:3:GLU:H	2.33	0.41
1:A:182:ILE:O	1:A:186:ILE:HG13	2.21	0.41
1:D:271:LEU:HB3	1:D:276:LEU:HD21	2.03	0.41
2:G:13:DG:H2"	2:G:14:DC:O5'	2.20	0.41
3:J:112:DT:C2'	3:J:113:DC:C6	3.04	0.41
1:B:503:LEU:O	1:B:504:HIS:C	2.58	0.41
1:A:119:SER:HA	1:A:120:PRO:HD3	1.93	0.41
1:B:374:LYS:C	1:B:376:GLN:N	2.73	0.41
1:B:202:LEU:HD11	1:B:241:ARG:HB3	2.02	0.41
1:D:421:ARG:HD2	1:D:476:THR:OG1	2.20	0.41
1:D:367:ALA:O	1:D:370:PHE:HB3	2.21	0.41
1:C:253:ILE:O	1:C:259:SER:HA	2.21	0.41
1:C:257:TYR:N	1:C:257:TYR:CD1	2.89	0.41
1:B:457:SER:HA	1:B:458:PRO:HD3	1.86	0.41
1:B:703:THR:OG1	1:B:704:GLY:N	2.53	0.41
2:E:7:DA:H2'	2:E:8:DT:H72	2.02	0.41
1:C:659:MET:O	1:C:663:ILE:HG13	2.20	0.41
1:B:776:TYR:CE2	1:B:854:ILE:HG22	2.56	0.41
1:D:62:PHE:N	1:D:62:PHE:CD1	2.89	0.41
1:D:597:ILE:CG1	1:D:683:MET:HE1	2.48	0.41
1:B:791:TYR:HE2	1:B:800:LYS:O	2.04	0.41
1:C:271:LEU:HD11	1:C:355:ILE:HG22	2.02	0.41
1:B:469:GLY:O	1:B:472:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:PHE:O	1:B:774:LEU:HB2	2.20	0.41
1:D:883:PHE:N	1:D:883:PHE:HD2	2.18	0.41
1:A:898:PHE:N	1:A:898:PHE:CD1	2.86	0.41
1:C:256:MET:SD	1:C:257:TYR:CE1	3.14	0.41
1:C:543:PHE:O	1:C:547:ARG:HB2	2.21	0.41
1:D:135:ALA:C	1:D:136:ILE:HG22	2.40	0.40
1:D:835:LEU:HD11	1:D:843:ASP:O	2.21	0.40
1:D:317:HIS:CE1	1:D:321:ILE:CD1	3.04	0.40
1:C:83:LEU:H	1:C:83:LEU:HD22	1.86	0.40
1:C:66:ARG:C	1:C:66:ARG:HD2	2.41	0.40
1:D:216:TRP:HZ3	1:D:288:TYR:O	2.03	0.40
1:D:171:GLN:HG2	1:D:319:ARG:HH22	1.85	0.40
1:C:518:TYR:CD1	1:C:518:TYR:N	2.89	0.40
1:B:85:MET:HE3	1:B:576:ARG:NH2	2.36	0.40
1:A:280:PHE:HD2	1:A:343:LEU:HD21	1.84	0.40
1:B:285:GLN:HG2	1:B:293:ILE:HD13	2.03	0.40
1:D:348:GLY:HA3	1:D:355:ILE:HD13	2.03	0.40
1:A:618:LEU:HD23	1:A:626:TYR:O	2.21	0.40
1:A:685:ARG:HG2	1:A:685:ARG:NH1	2.37	0.40
1:C:540:GLU:HA	1:C:540:GLU:OE1	2.21	0.40
1:B:137:THR:HG22	1:B:328:VAL:HG21	2.02	0.40
1:C:484:GLU:HG2	1:C:488:TYR:CE2	2.56	0.40
1:B:71:TRP:NE1	1:B:75:MET:HE2	2.36	0.40
1:D:769:LYS:O	1:D:773:GLN:NE2	2.54	0.40
1:A:268:ILE:CG2	1:A:269:SER:N	2.84	0.40
1:C:703:THR:HG22	1:C:886:ALA:CB	2.52	0.40
1:A:362:ILE:HG12	1:A:572:ASN:HD21	1.80	0.40
1:B:508:LEU:CD2	1:B:508:LEU:H	2.23	0.40
1:A:553:MET:O	1:A:556:GLN:HG3	2.21	0.40
1:A:207:GLN:C	1:A:208:LYS:HG3	2.41	0.40
1:A:218:VAL:CG2	1:A:223:ILE:HG13	2.52	0.40
1:D:750:ARG:NH2	1:D:755:GLU:OE1	2.54	0.40
1:B:89:LYS:HE3	1:B:354:GLN:NE2	2.36	0.40
1:A:432:GLY:O	1:A:462:MET:N	2.55	0.40
1:C:253:ILE:HD13	2:I:1:DC:C5	2.56	0.40
1:D:887:ALA:O	1:D:888:LYS:HB2	2.21	0.40
1:B:433:THR:HA	1:B:460:GLY:O	2.21	0.40
1:D:202:LEU:C	1:D:202:LEU:HD23	2.41	0.40
3:F:106:DT:H1'	3:F:107:DG:C5'	2.44	0.40
1:A:502:ALA:C	1:A:503:LEU:HD12	2.41	0.40
1:B:223:ILE:HB	1:B:224:PRO:CD	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:SER:O	1:C:541:MET:HG3	2.22	0.40
1:A:546:GLN:HA	1:A:549:GLU:HB2	2.03	0.40
1:D:458:PRO:HB2	1:D:588:THR:HG22	2.02	0.40
1:C:273:TYR:CE2	1:C:335:ASP:HB2	2.57	0.40
1:B:252:VAL:O	1:B:253:ILE:C	2.59	0.40
3:H:110:DA:H1'	3:H:111:DT:H5"	2.02	0.40
1:D:303:LEU:O	1:D:304:LYS:C	2.59	0.40
1:A:113:PHE:CE1	1:A:218:VAL:CG2	3.05	0.40
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.97	0.40
1:A:221:PHE:C	1:A:224:PRO:HD2	2.42	0.40
1:A:338:ARG:HG3	1:A:338:ARG:NH1	2.36	0.40
1:C:42:PRO:O	1:C:43:GLU:C	2.59	0.40
1:D:456:CYS:HA	1:D:461:MET:O	2.21	0.40
1:D:659:MET:O	1:D:660:GLU:C	2.59	0.40
1:D:291:ASP:O	1:D:292:TYR:C	2.60	0.40
1:C:582:ASN:O	1:C:585:ALA:HB3	2.21	0.40
1:B:626:TYR:CD1	1:B:626:TYR:N	2.89	0.40
1:D:546:GLN:O	1:D:549:GLU:HB3	2.22	0.40
1:C:393:GLY:O	1:C:587:THR:HG23	2.22	0.40
1:C:514:LEU:CD2	1:C:526:ILE:HG23	2.51	0.40
1:B:326:ILE:O	1:B:330:ARG:CG	2.66	0.40
1:B:117:VAL:HG11	1:B:225:TYR:OH	2.21	0.40
1:D:318:GLN:O	1:D:322:SER:HB2	2.21	0.40
1:C:332:LEU:O	1:C:336:ALA:HB2	2.22	0.40
1:B:837:GLU:CG	1:B:838:GLY:H	2.34	0.40
1:C:365:TRP:CD2	1:C:566:LEU:HD13	2.56	0.40
1:A:410:PHE:HB2	1:A:683:MET:CE	2.51	0.40
1:D:302:LYS:HD2	1:D:302:LYS:N	2.37	0.40
1:C:503:LEU:HD21	1:C:538:LEU:HB2	2.03	0.40
1:A:106:THR:HG22	1:A:106:THR:O	2.20	0.40
1:B:355:ILE:HD13	1:B:355:ILE:HA	1.90	0.40
1:B:443:ILE:HD13	1:B:595:GLN:CB	2.51	0.40
1:D:468:ASP:OD2	1:D:677:LYS:HE2	2.22	0.40
1:C:651:LEU:HA	1:C:651:LEU:HD23	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	900/906 (99%)	745 (83%)	129 (14%)	26 (3%)	6	29
1	B	900/906 (99%)	761 (85%)	119 (13%)	20 (2%)	8	38
1	C	899/906 (99%)	748 (83%)	125 (14%)	26 (3%)	6	29
1	D	886/906 (98%)	710 (80%)	133 (15%)	43 (5%)	3	16
All	All	3585/3624 (99%)	2964 (83%)	506 (14%)	115 (3%)	5	27

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	A	790	LYS
1	A	863	LEU
1	B	819	ILE
1	C	177	GLU
1	D	181	GLU
1	D	187	ILE
1	D	192	ASP
1	D	524	ASP
1	D	855	THR
1	A	105	HIS
1	A	169	LYS
1	A	283	THR
1	A	521	ASP
1	A	613	GLY
1	A	772	ARG
1	A	776	TYR
1	A	836	ARG
1	A	841	PHE
1	B	187	ILE
1	B	352	LYS
1	B	392	PRO

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Mol	Chain	Res	Type
1	C	172	GLU
1	C	179	PRO
1	C	315	SER
1	C	790	LYS
1	D	43	GLU
1	D	45	GLN
1	D	96	THR
1	D	272	ASP
1	D	508	LEU
1	D	534	SER
1	D	814	ALA
1	D	822	PRO
1	D	865	TRP
1	A	46	ALA
1	A	738	PRO
1	A	893	LYS
1	B	236	GLU
1	B	237	SER
1	B	375	GLU
1	C	98	ASN
1	C	170	LEU
1	C	314	GLU
1	C	320	TYR
1	C	622	THR
1	D	21	ASP
1	D	44	SER
1	D	98	ASN
1	D	222	ALA
1	D	483	LYS
1	D	532	LYS
1	D	574	TRP
1	D	730	LEU
1	A	394	ALA
1	A	518	TYR
1	A	655	ALA
1	A	898	PHE
1	B	99	TYR
1	B	222	ALA
1	B	252	VAL
1	B	344	SER
1	B	526	ILE
1	B	828	GLU

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Mol	Chain	Res	Type
1	C	222	ALA
1	C	303	LEU
1	C	310	SER
1	C	415	LEU
1	C	514	LEU
1	C	534	SER
1	D	64	ASN
1	D	161	GLU
1	D	186	ILE
1	D	435	LYS
1	D	459	ASN
1	D	528	GLU
1	D	622	THR
1	D	836	ARG
1	A	622	THR
1	A	802	PRO
1	B	300	VAL
1	B	504	HIS
1	B	802	PRO
1	C	430	ILE
1	C	593	ALA
1	C	814	ALA
1	D	240	LYS
1	D	304	LYS
1	D	450	PRO
1	D	512	GLU
1	D	531	LYS
1	D	570	LEU
1	D	630	ASP
1	D	810	THR
1	C	144	ASP
1	C	155	PRO
1	C	414	SER
1	D	300	VAL
1	D	414	SER
1	D	460	GLY
1	D	723	PRO
1	B	142	ILE
1	C	458	PRO
1	D	136	ILE
1	C	510	VAL
1	A	848	TRP

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Mol	Chain	Res	Type
1	B	307	GLY
1	C	840	PRO
1	A	450	PRO
1	B	499	ILE
1	C	608	VAL
1	A	250	VAL
1	A	526	ILE
1	A	608	VAL
1	B	125	GLU

5.3.2 Protein sidechains (i)

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	789/803 (98%)	715 (91%)	74 (9%)	11	39
1	B	773/803 (96%)	717 (93%)	56 (7%)	18	53
1	C	794/803 (99%)	745 (94%)	49 (6%)	23	60
1	D	737/803 (92%)	672 (91%)	65 (9%)	12	42
All	All	3093/3212 (96%)	2849 (92%)	244 (8%)	15	48

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	PHE
1	A	25	ARG
1	A	28	THR
1	A	29	ARG
1	A	36	SER
1	A	43	GLU
1	A	58	THR
1	A	59	ARG
1	A	61	LEU
1	A	64	ASN
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	86	ASP
1	A	94	SER
1	A	98	ASN
1	A	105	HIS
1	A	138	HIS
1	A	140	ASP
1	A	196	GLU
1	A	213	LEU
1	A	220	SER
1	A	229	ARG
1	A	242	LEU
1	A	260	ARG
1	A	280	PHE
1	A	285	GLN
1	A	292	TYR
1	A	298	LEU
1	A	304	LYS
1	A	314	GLU
1	A	318	GLN
1	A	339	GLN
1	A	342	ASN
1	A	347	MET
1	A	372	SER
1	A	379	VAL
1	A	408	MET
1	A	410	PHE
1	A	433	THR
1	A	466	ASP
1	A	467	ARG
1	A	475	ILE
1	A	479	PHE
1	A	498	ILE
1	A	543	PHE
1	A	544	ARG
1	A	546	GLN
1	A	548	THR
1	A	556	GLN
1	A	559	ARG
1	A	561	LEU
1	A	587	THR
1	A	602	ASN
1	A	612	GLU

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Mol	Chain	Res	Type
1	A	618	LEU
1	A	653	LYS
1	A	658	ARG
1	A	703	THR
1	A	708	TYR
1	A	731	GLU
1	A	735	SER
1	A	745	LEU
1	A	754	GLN
1	A	758	GLU
1	A	773	GLN
1	A	776	TYR
1	A	806	ARG
1	A	813	ARG
1	A	824	VAL
1	A	846	ILE
1	A	861	ASP
1	A	873	GLU
1	A	880	LEU
1	A	893	LYS
1	B	9	GLU
1	B	22	SER
1	B	47	THR
1	B	61	LEU
1	B	83	LEU
1	B	86	ASP
1	B	90	LEU
1	B	113	PHE
1	B	115	ILE
1	B	116	GLU
1	B	130	LYS
1	B	145	ARG
1	B	146	PHE
1	B	147	TYR
1	B	164	ILE
1	B	177	GLU
1	B	181	GLU
1	B	218	VAL
1	B	248	THR
1	B	249	ARG
1	B	257	TYR
1	B	260	ARG

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Mol	Chain	Res	Type
1	B	274	ILE
1	B	280	PHE
1	B	291	ASP
1	B	316	ASN
1	B	377	ASN
1	B	378	LYS
1	B	386	HIS
1	B	392	PRO
1	B	421	ARG
1	B	451	SER
1	B	468	ASP
1	B	475	ILE
1	B	479	PHE
1	B	489	MET
1	B	495	ASN
1	B	499	ILE
1	B	570	LEU
1	B	632	ILE
1	B	658	ARG
1	B	668	ARG
1	B	685	ARG
1	B	686	GLU
1	B	702	TRP
1	B	708	TYR
1	B	728	MET
1	B	742	GLN
1	B	758	GLU
1	B	766	GLU
1	B	773	GLN
1	B	843	ASP
1	B	856	ASP
1	B	860	ASP
1	B	891	TYR
1	B	899	ASP
1	C	7	THR
1	C	25	ARG
1	C	58	THR
1	C	60	LYS
1	C	61	LEU
1	C	66	ARG
1	C	93	LEU
1	C	138	HIS

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Mol	Chain	Res	Type
1	C	149	PHE
1	C	173	GLN
1	C	192	ASP
1	C	195	LYS
1	C	196	GLU
1	C	200	GLU
1	C	214	THR
1	C	231	LYS
1	C	255	ASN
1	C	256	MET
1	C	257	TYR
1	C	261	GLU
1	C	276	LEU
1	C	284	ASN
1	C	302	LYS
1	C	388	VAL
1	C	399	PRO
1	C	428	GLU
1	C	439	LEU
1	C	473	THR
1	C	474	GLU
1	C	490	LEU
1	C	525	GLU
1	C	556	GLN
1	C	559	ARG
1	C	561	LEU
1	C	562	LEU
1	C	587	THR
1	C	618	LEU
1	C	640	LYS
1	C	642	ARG
1	C	667	PHE
1	C	702	TRP
1	C	731	GLU
1	C	760	LEU
1	C	765	LYS
1	C	770	GLU
1	C	843	ASP
1	C	856	ASP
1	C	880	LEU
1	C	898	PHE
1	D	1	MET

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Mol	Chain	Res	Type
1	D	10	GLN
1	D	13	ASP
1	D	32	GLU
1	D	41	CYS
1	D	57	CYS
1	D	67	ASP
1	D	86	ASP
1	D	102	LYS
1	D	105	HIS
1	D	113	PHE
1	D	128	GLN
1	D	136	ILE
1	D	152	LEU
1	D	156	TYR
1	D	164	ILE
1	D	182	ILE
1	D	197	LEU
1	D	198	LEU
1	D	200	GLU
1	D	202	LEU
1	D	208	LYS
1	D	213	LEU
1	D	216	TRP
1	D	221	PHE
1	D	225	TYR
1	D	273	TYR
1	D	285	GLN
1	D	302	LYS
1	D	305	TYR
1	D	310	SER
1	D	362	ILE
1	D	363	LYS
1	D	407	VAL
1	D	452	ASP
1	D	456	CYS
1	D	474	GLU
1	D	479	PHE
1	D	484	GLU
1	D	485	HIS
1	D	511	ASP
1	D	518	TYR
1	D	520	PHE

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Mol	Chain	Res	Type
1	D	524	ASP
1	D	540	GLU
1	D	558	ASN
1	D	576	ARG
1	D	591	GLN
1	D	592	MET
1	D	618	LEU
1	D	630	ASP
1	D	658	ARG
1	D	660	GLU
1	D	667	PHE
1	D	674	MET
1	D	702	TRP
1	D	710	LEU
1	D	725	LEU
1	D	731	GLU
1	D	779	ILE
1	D	812	ASN
1	D	839	ASN
1	D	844	LYS
1	D	852	THR
1	D	873	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	23	ASN
1	A	40	HIS
1	A	64	ASN
1	A	112	ASN
1	A	153	ASN
1	A	171	GLN
1	A	255	ASN
1	A	285	GLN
1	A	342	ASN
1	A	389	GLN
1	A	422	GLN
1	A	495	ASN
1	A	505	ASN
1	A	546	GLN
1	A	556	GLN

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Mol	Chain	Res	Type
1	A	602	ASN
1	A	606	ASN
1	A	646	HIS
1	A	678	GLN
1	A	733	GLN
1	A	773	GLN
1	A	786	ASN
1	A	812	ASN
1	A	818	ASN
1	A	864	HIS
1	B	128	GLN
1	B	138	HIS
1	B	171	GLN
1	B	173	GLN
1	B	193	ASN
1	B	206	GLN
1	B	245	HIS
1	B	284	ASN
1	B	318	GLN
1	B	354	GLN
1	B	376	GLN
1	B	382	GLN
1	B	389	GLN
1	B	495	ASN
1	B	505	ASN
1	B	539	ASN
1	B	556	GLN
1	B	558	ASN
1	B	591	GLN
1	B	646	HIS
1	B	733	GLN
1	B	742	GLN
1	B	754	GLN
1	B	773	GLN
1	B	775	ASN
1	B	812	ASN
1	B	818	ASN
1	C	45	GLN
1	C	128	GLN
1	C	171	GLN
1	C	193	ASN
1	C	255	ASN

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Mol	Chain	Res	Type
1	C	284	ASN
1	C	285	GLN
1	C	318	GLN
1	C	440	HIS
1	C	444	ASN
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	646	HIS
1	C	675	ASN
1	C	678	GLN
1	C	711	ASN
1	C	761	GLN
1	C	787	ASN
1	C	818	ASN
1	D	70	GLN
1	D	128	GLN
1	D	171	GLN
1	D	206	GLN
1	D	207	GLN
1	D	245	HIS
1	D	285	GLN
1	D	317	HIS
1	D	318	GLN
1	D	324	ASN
1	D	354	GLN
1	D	382	GLN
1	D	480	ASN
1	D	495	ASN
1	D	505	ASN
1	D	539	ASN
1	D	546	GLN
1	D	676	ASN
1	D	679	HIS
1	D	733	GLN
1	D	742	GLN
1	D	754	GLN
1	D	773	GLN
1	D	812	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CTG	E	4	3,2	16,23,24	0.81	1 (6%)	17,35,38	1.10	2 (11%)
2	CTG	G	4	3,2	16,23,24	0.82	1 (6%)	17,35,38	1.22	2 (11%)
2	CTG	I	4	3,2	16,23,24	0.97	1 (6%)	17,35,38	1.33	3 (17%)

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	E	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	G	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	I	4	3,2	-	0/7/45/46	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	CTG	C1'-N1	2.17	1.48	1.45
2	E	4	CTG	C1'-N1	2.32	1.48	1.45
2	I	4	CTG	C1'-N1	2.64	1.49	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	CTG	C2'-C1'-N1	-3.58	110.74	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	CTG	C2'-C1'-N1	-3.29	111.13	115.64
2	G	4	CTG	C2'-C1'-N1	-3.22	111.23	115.64
2	G	4	CTG	N3-C2-N1	-2.71	114.11	116.82
2	I	4	CTG	N3-C2-N1	-2.36	114.46	116.82
2	E	4	CTG	N3-C2-N1	-2.17	114.65	116.82
2	I	4	CTG	C2'-C3'-C4'	2.04	107.00	102.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	CTG	3	0
2	G	4	CTG	4	0
2	I	4	CTG	4	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^{th} 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^2)	Q<0.9
1	A	902/906 (99%)	-0.11	26 (2%) 55 26	29, 63, 155, 176	0
1	B	902/906 (99%)	0.21	70 (7%) 16 6	30, 84, 172, 189	2 (0%)
1	C	901/906 (99%)	-0.21	7 (0%) 87 67	23, 64, 127, 148	0
1	D	890/906 (98%)	0.32	65 (7%) 18 6	72, 132, 174, 188	3 (0%)
2	E	17/18 (94%)	0.19	0 100 100	75, 106, 144, 148	0
2	G	17/18 (94%)	0.21	0 100 100	76, 113, 137, 147	0
2	I	17/18 (94%)	-0.23	0 100 100	39, 53, 124, 140	0
2	K	14/18 (77%)	0.58	1 (7%) 19 7	69, 156, 169, 170	0
3	F	14/14 (100%)	-0.07	0 100 100	85, 125, 157, 161	0
3	H	14/14 (100%)	-0.05	0 100 100	89, 132, 155, 156	0
3	J	14/14 (100%)	-0.53	0 100 100	35, 55, 123, 127	0
3	L	13/14 (92%)	0.55	1 (7%) 16 6	146, 165, 169, 175	0
All	All	3715/3752 (99%)	0.05	170 (4%) 36 14	23, 83, 165, 189	5 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	HIS	8.2
1	D	847	ALA	7.8
1	D	862	VAL	7.7
1	D	535	ALA	6.5
1	B	510	VAL	6.2
1	B	503	LEU	6.2
1	B	819	ILE	5.9
1	D	858	ILE	5.7
1	D	857	LEU	5.5
1	D	802	PRO	5.5
1	B	505	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	508	LEU	5.3
1	B	506	PRO	5.2
1	B	865	TRP	5.2
1	D	793	VAL	5.2
1	A	498	ILE	4.8
1	B	516	VAL	4.7
1	B	793	VAL	4.6
1	B	511	ASP	4.5
1	B	846	ILE	4.5
1	B	513	PRO	4.5
1	B	522	PHE	4.5
1	D	851	GLY	4.4
1	B	315	SER	4.3
1	B	821	ALA	4.3
1	D	534	SER	4.3
1	B	303	LEU	4.3
1	A	514	LEU	4.3
1	B	523	SER	4.2
1	D	834	PRO	4.1
1	B	509	SER	4.0
1	D	855	THR	4.0
1	B	542	LEU	3.8
1	B	306	ASP	3.7
1	D	819	ILE	3.7
1	D	863	LEU	3.7
1	B	160	GLU	3.7
1	B	502	ALA	3.7
1	A	513	PRO	3.7
1	D	510	VAL	3.6
1	B	134	ASP	3.6
1	D	833	LEU	3.6
1	D	794	GLY	3.5
1	D	778	SER	3.5
1	B	307	GLY	3.4
1	B	532	LYS	3.4
1	B	798	GLY	3.4
1	D	393	GLY	3.4
1	B	128	GLN	3.3
1	B	803	PHE	3.3
1	D	801	CYS	3.3
1	B	817	GLY	3.3
1	D	511	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	498	ILE	3.2
1	B	173	GLN	3.2
1	B	818	ASN	3.2
1	D	771	PHE	3.2
1	D	846	ILE	3.2
1	D	504	HIS	3.2
1	B	286	PRO	3.2
1	B	174	GLY	3.1
1	D	849	PRO	3.1
1	B	129	ALA	3.1
1	C	303	LEU	3.1
1	A	505	ASN	3.1
1	B	530	ILE	3.0
1	D	120	PRO	3.0
3	L	113	DC	3.0
1	D	792	ASP	3.0
1	D	522	PHE	3.0
1	B	492	ALA	3.0
1	D	818	ASN	2.9
1	D	831	TYR	2.9
1	D	395	PHE	2.9
1	A	504	HIS	2.9
1	D	192	ASP	2.9
1	A	808	ILE	2.9
1	B	861	ASP	2.9
1	D	832	VAL	2.9
1	A	786	ASN	2.9
1	B	507	ASN	2.9
1	B	862	VAL	2.8
1	A	508	LEU	2.8
1	A	855	THR	2.8
1	C	513	PRO	2.8
1	B	813	ARG	2.8
1	D	523	SER	2.8
1	B	155	PRO	2.8
1	C	498	ILE	2.7
1	D	505	ASN	2.7
1	B	499	ILE	2.7
1	C	508	LEU	2.7
2	K	6	DA	2.7
1	A	506	PRO	2.7
1	A	526	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	179	PRO	2.7
1	D	183	ILE	2.7
1	D	542	LEU	2.6
1	B	127	SER	2.6
1	B	501	GLU	2.6
1	B	526	ILE	2.6
1	B	157	GLY	2.6
1	D	788	ILE	2.6
1	A	524	ASP	2.6
1	D	856	ASP	2.6
1	A	841	PHE	2.6
1	D	248	THR	2.6
1	A	858	ILE	2.6
1	B	514	LEU	2.6
1	A	512	GLU	2.6
1	D	286	PRO	2.5
1	D	10	GLN	2.5
1	A	820	ASP	2.5
1	B	539	ASN	2.5
1	D	266	PHE	2.5
1	D	820	ASP	2.5
1	A	776	TYR	2.5
1	B	153	ASN	2.5
1	B	340	PHE	2.5
1	D	507	ASN	2.4
1	D	391	TYR	2.4
1	D	848	TRP	2.4
1	D	817	GLY	2.4
1	D	774	LEU	2.4
1	D	173	GLN	2.4
1	B	797	PRO	2.3
1	A	515	ASP	2.3
1	B	175	GLY	2.3
1	A	863	LEU	2.3
1	B	535	ALA	2.3
1	B	820	ASP	2.3
1	D	850	SER	2.3
1	B	546	GLN	2.3
1	D	786	ASN	2.3
1	B	521	ASP	2.3
1	B	868	TYR	2.3
1	B	497	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	792	ASP	2.2
1	B	799	PRO	2.2
1	C	173	GLN	2.2
1	A	254	GLU	2.2
1	D	812	ASN	2.2
1	D	499	ILE	2.2
1	D	539	ASN	2.1
1	D	514	LEU	2.1
1	D	546	GLN	2.1
1	D	135	ALA	2.1
1	C	506	PRO	2.1
1	D	394	ALA	2.1
1	D	157	GLY	2.1
1	D	133	ILE	2.1
1	A	501	GLU	2.1
1	B	538	LEU	2.1
1	A	532	LYS	2.1
1	B	166	ILE	2.1
1	A	787	ASN	2.1
1	D	543	PHE	2.1
1	D	777	ILE	2.0
1	B	512	GLU	2.0
1	B	528	GLU	2.0
1	D	175	GLY	2.0
1	A	847	ALA	2.0
1	B	234	PHE	2.0
1	C	522	PHE	2.0
1	D	113	PHE	2.0
1	B	118	THR	2.0
1	D	162	TRP	2.0
1	A	537	SER	2.0
1	B	541	MET	2.0
1	A	819	ILE	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CTG	E	4	22/23	0.86	0.22	-	109,113,124,125	0
2	CTG	G	4	22/23	0.74	0.27	-	122,128,129,129	0
2	CTG	I	4	22/23	0.93	0.21	-	72,78,81,81	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.