



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:49 AM UTC

PDB ID : 3RMD / pdb_00003rmd
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing
Thymine Glycol
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.
Deposited on : 2011-04-20
Resolution : 2.98 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

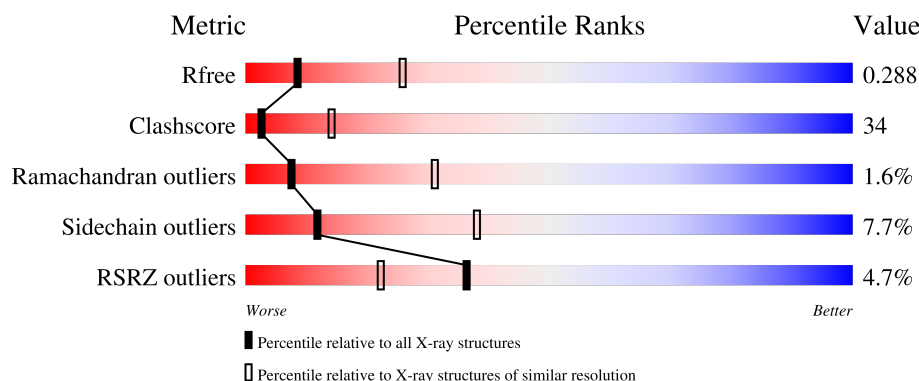
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	906	
1	B	906	
1	C	906	
1	D	906	
2	E	18	

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Mol	Chain	Length	Quality of chain
2	G	18	39% 50% 11%
2	I	18	11% 83% 6%
2	K	18	17% 78% 6%
3	F	15	13% 40% 47% 13%
3	H	15	7% 47% 53%
3	J	15	13% 73% 13%
3	L	15	20% 80%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31870 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
			7284	4679	1208	1365	32			
1	B	902	Total	C	N	O	S	0	0	0
			7315	4695	1216	1371	33			
1	C	901	Total	C	N	O	S	0	0	0
			7312	4695	1212	1372	33			
1	D	897	Total	C	N	O	S	3	0	0
			7165	4599	1184	1350	32			

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

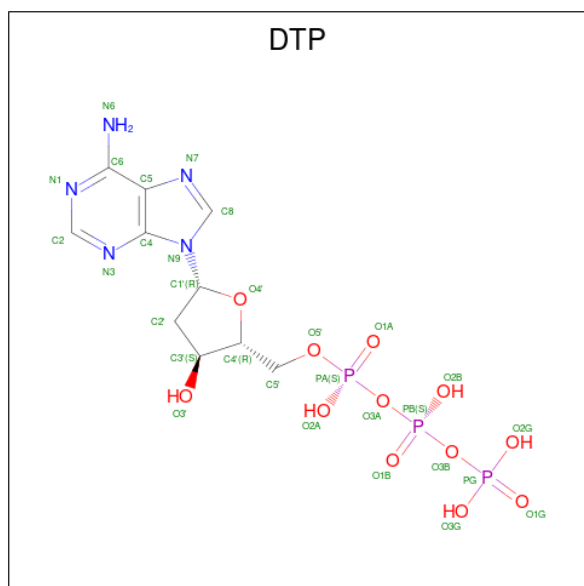
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			265	126	54	73	12			
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	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			
3	H	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
3	J	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
3	L	15	Total	C	N	O	P	0	0	0
			301	143	55	89	14			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	J	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

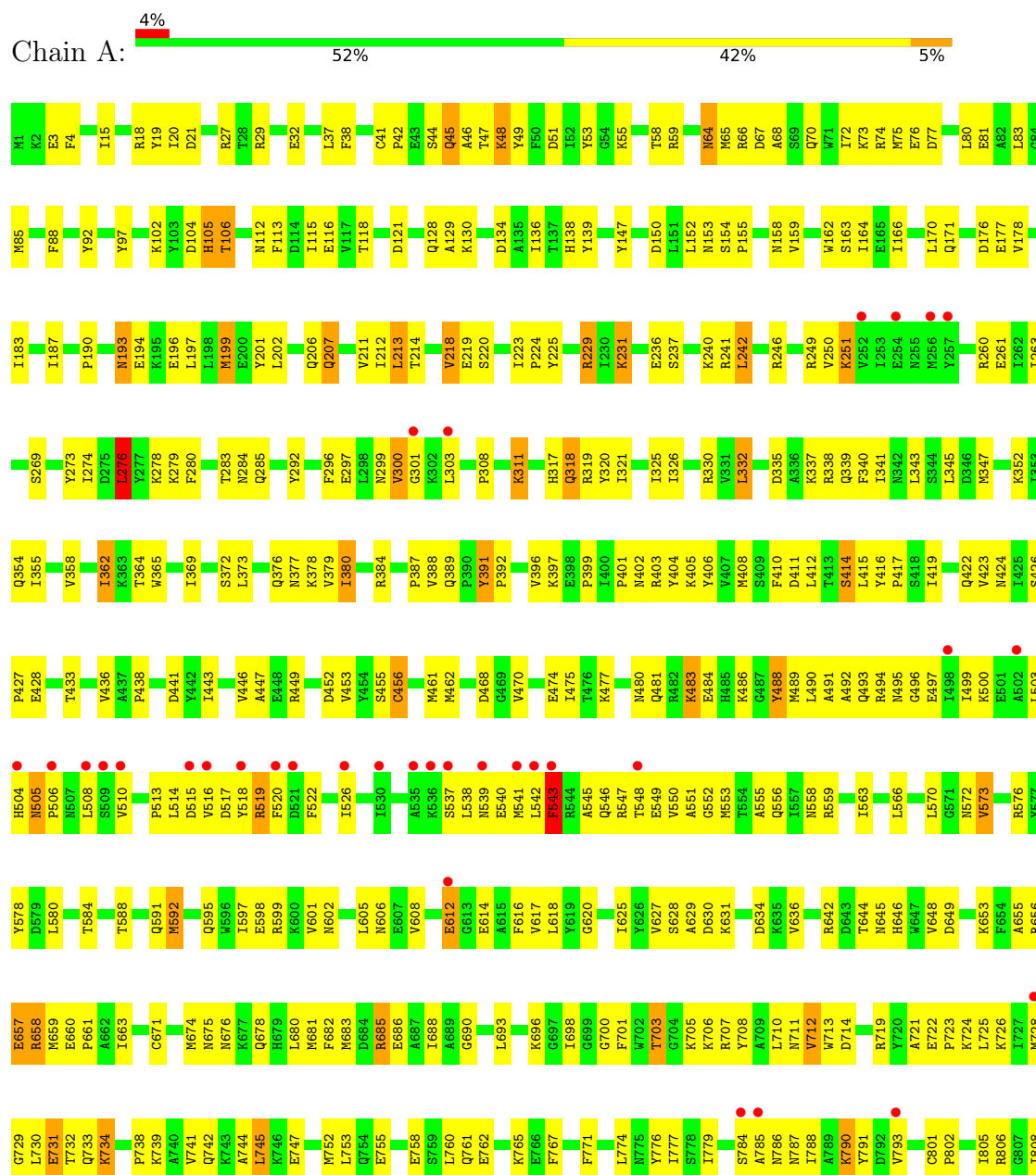
- Molecule 5 is water.

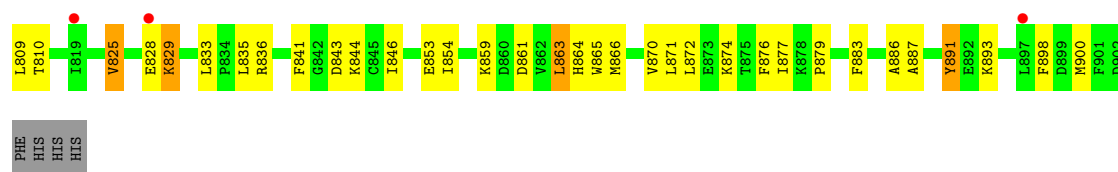
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	50	Total	O	0	0
			50	50		
5	C	40	Total	O	0	0
			40	40		
5	D	27	Total	O	0	0
			27	27		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	G	2	Total	O	0	0
			2	2		
5	H	1	Total	O	0	0
			1	1		
5	I	3	Total	O	0	0
			3	3		
5	J	2	Total	O	0	0
			2	2		
5	K	1	Total	O	0	0
			1	1		
5	L	1	Total	O	0	0
			1	1		

3 Residue-property plots

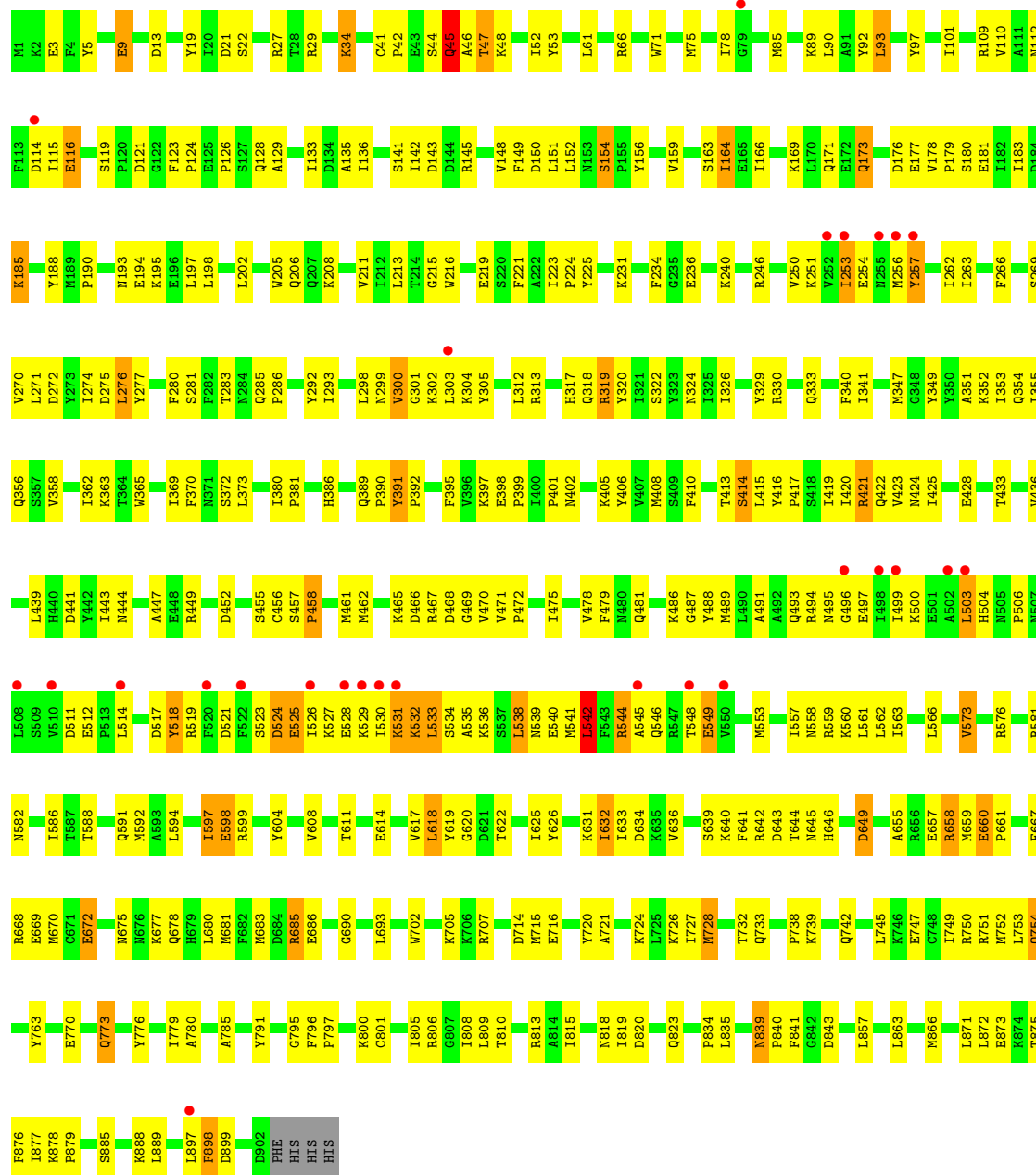
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase



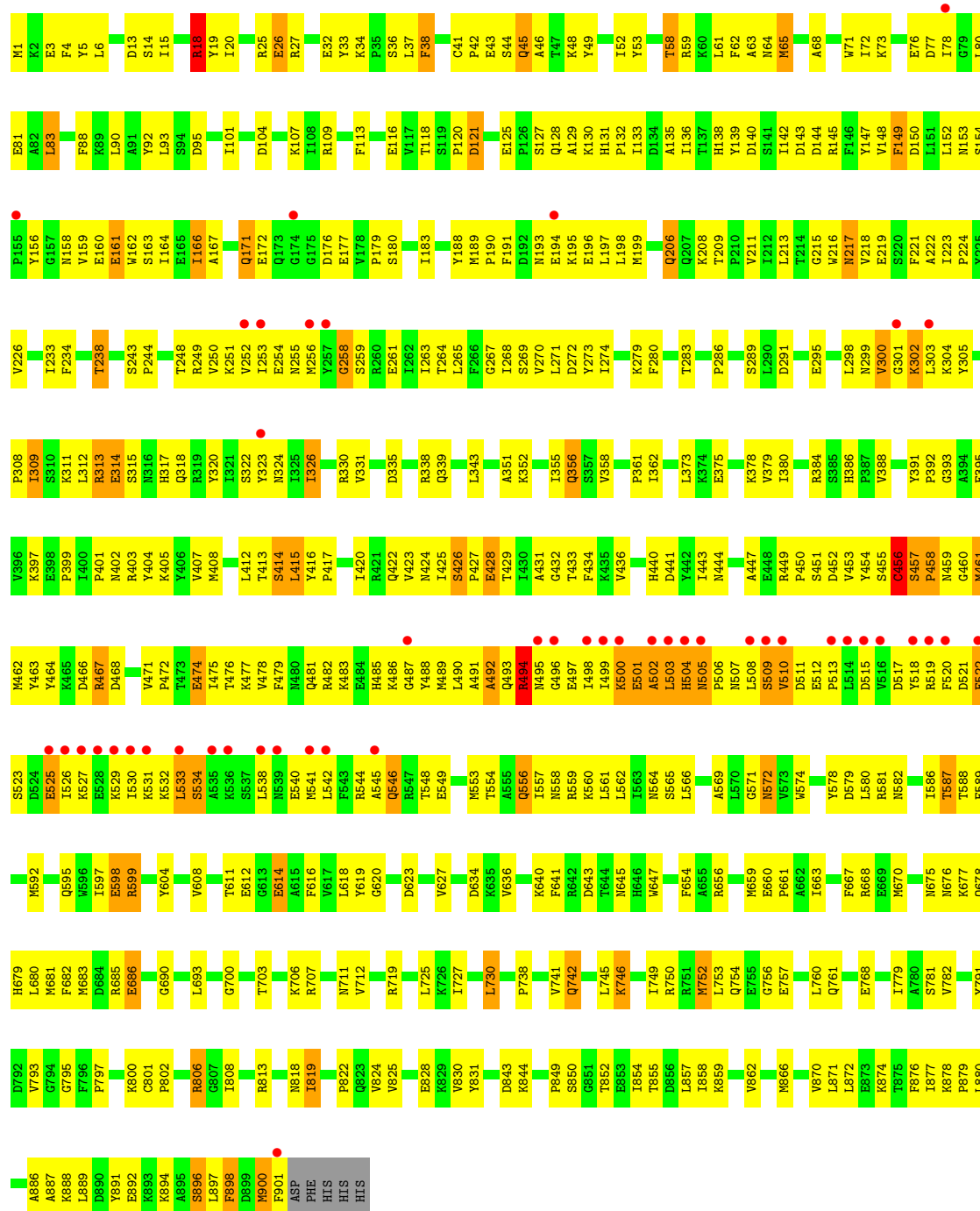


- Molecule 1: DNA polymerase



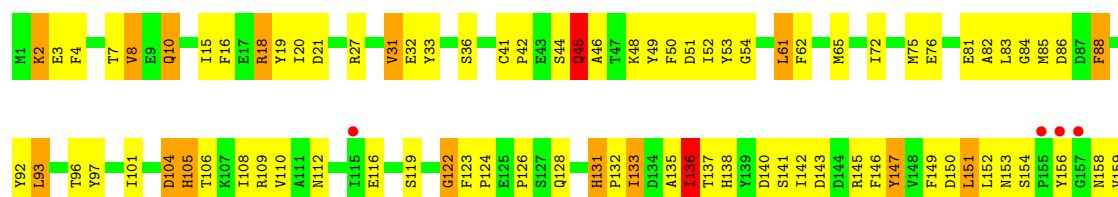
- Molecule 1: DNA polymerase





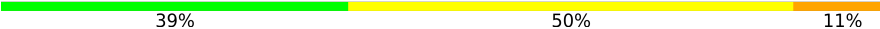
• Molecule 1: DNA polymerase

Chain D: 7% 38% 52% 9% ..



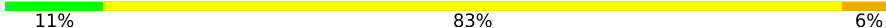


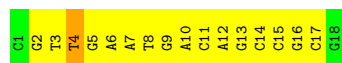
WORLD WIDE
PDB
PROTEIN DATA BANK

Chain G:  39% 50% 11%

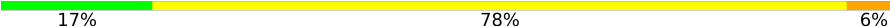


- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:  11% 83% 6%



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

Chain K:  17% 78% 6%



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

Chain F:  13% 40% 47% 13%

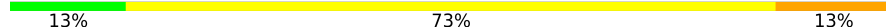


- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*AP*A)-3')

Chain H:  7% 47% 53%



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

Chain J:  13% 73% 13%



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

Chain L:  20% 80%

G101	G103
C102	G104
	C105
	T106
	G107
	T108
	C109
	A110
	T111
	T112
	C113
	A114
	A115

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.84Å 123.03Å 168.78Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 50.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-2.98) 93.7 (50.00-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.275 0.235 , 0.288	Depositor DCC
R_{free} test set	20372 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31870	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTG, DTP

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	0.58	0/7462	0.98	28/10099 (0.3%)
1	B	0.53	0/7494	0.98	23/10138 (0.2%)
1	C	0.55	0/7491	0.99	32/10134 (0.3%)
1	D	0.47	0/7343	0.98	32/9963 (0.3%)
2	E	0.29	0/298	0.59	0/458
2	G	0.32	0/390	0.79	1/598 (0.2%)
2	I	0.39	0/390	0.75	0/598
2	K	0.29	0/390	0.60	1/598 (0.2%)
3	F	0.36	0/292	0.66	0/449
3	H	0.32	0/340	0.74	0/523
3	J	0.34	0/340	0.93	3/523 (0.6%)
3	L	0.29	0/337	0.66	0/517
All	All	0.52	0/32567	0.96	120/44598 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-9.76	102.40	111.67
1	D	122	GLY	N-CA-C	-9.62	102.23	112.04
1	B	211	VAL	N-CA-C	-9.62	102.53	111.67
1	C	501	GLU	N-CA-C	-9.11	101.70	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	115	DA	C2'-C3'-O3'	8.03	123.55	111.50
1	B	598	GLU	N-CA-C	-7.87	102.65	111.07
1	D	542	LEU	N-CA-C	-7.64	103.98	113.38
1	D	391	TYR	N-CA-C	7.55	121.76	109.15
1	B	504	HIS	N-CA-C	-7.31	104.36	113.28
1	A	729	GLY	N-CA-C	7.02	124.33	115.21
1	C	598	GLU	N-CA-C	-6.89	103.70	111.07
1	C	504	HIS	N-CA-C	-6.77	106.22	114.75
1	B	457	SER	CA-C-N	6.72	128.25	119.84
1	B	457	SER	C-N-CA	6.72	128.25	119.84
2	G	18	DG	C2'-C3'-O3'	-6.57	101.64	111.50
1	D	391	TYR	CA-CB-CG	6.49	125.59	113.90
1	A	436	VAL	N-CA-C	6.47	118.13	108.23
1	C	171	GLN	N-CA-C	6.47	119.32	111.82
3	J	114	DA	C2'-C3'-O3'	6.42	121.12	111.50
1	D	391	TYR	N-CA-CB	-6.38	98.62	110.05
1	A	721	ALA	N-CA-C	-6.37	104.26	111.14
1	B	754	GLN	N-CA-C	6.35	121.05	113.12
1	C	500	LYS	N-CA-C	-6.31	105.89	113.97
1	D	201	TYR	N-CA-C	-6.28	104.36	111.14
1	A	657	GLU	N-CA-C	6.21	118.13	111.36
1	C	756	GLY	N-CA-C	6.21	119.84	112.33
1	C	546	GLN	N-CA-C	-6.16	104.49	112.68
1	D	598	GLU	N-CA-C	-6.13	104.52	111.07
1	B	121	ASP	N-CA-C	6.08	120.57	111.81
1	D	131	HIS	CA-C-N	6.08	126.09	119.89
1	D	131	HIS	C-N-CA	6.08	126.09	119.89
1	A	488	TYR	N-CA-C	-5.97	105.75	113.16
1	A	543	PHE	N-CA-C	-5.97	103.45	112.04
1	C	18	ARG	N-CA-C	-5.97	99.98	109.59
1	C	502	ALA	N-CA-C	-5.95	105.33	113.30
1	B	742	GLN	N-CA-C	-5.92	104.83	111.28
3	J	115	DA	C4'-C3'-O3'	5.92	118.87	110.00
1	C	436	VAL	N-CA-C	5.89	117.25	108.23
1	C	289	SER	N-CA-C	-5.89	102.20	110.50
1	A	486	LYS	N-CA-C	-5.87	106.09	113.20
1	B	391	TYR	CA-C-N	5.85	126.19	119.93
1	B	391	TYR	C-N-CA	5.85	126.19	119.93
1	C	503	LEU	N-CA-C	-5.85	105.96	112.57
1	A	276	LEU	N-CA-C	-5.84	104.60	110.97
1	D	390	PRO	CA-C-N	5.83	132.60	122.28
1	D	390	PRO	C-N-CA	5.83	132.60	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	LEU	N-CA-C	-5.81	104.63	110.97
1	D	436	VAL	N-CA-C	5.78	117.07	108.23
1	A	55	LYS	CA-C-N	5.75	125.51	119.76
1	A	55	LYS	C-N-CA	5.75	125.51	119.76
1	C	742	GLN	N-CA-C	-5.72	105.04	111.28
1	D	496	GLY	N-CA-C	-5.71	107.83	115.32
1	D	743	LYS	N-CA-C	-5.71	106.66	113.97
1	B	496	GLY	N-CA-C	-5.70	106.76	115.66
1	B	839	ASN	CA-C-N	5.70	126.97	119.84
1	B	839	ASN	C-N-CA	5.70	126.97	119.84
1	D	806	ARG	N-CA-C	-5.68	104.78	110.97
1	A	877	ILE	N-CA-C	5.66	116.11	110.23
1	A	891	TYR	N-CA-C	-5.65	106.05	113.17
1	D	558	ASN	N-CA-C	-5.62	105.68	112.54
1	A	598	GLU	N-CA-C	-5.61	105.06	111.07
1	D	88	PHE	N-CA-C	5.61	117.39	111.28
1	A	456	CYS	N-CA-C	5.57	118.33	109.81
1	C	309	ILE	CB-CA-C	-5.54	104.88	111.97
1	B	456	CYS	N-CA-C	5.53	118.28	109.81
1	D	735	SER	N-CA-C	-5.53	106.67	113.41
1	C	166	ILE	CB-CA-C	-5.53	104.59	112.22
1	A	18	ARG	N-CA-C	-5.52	99.91	108.90
1	B	215	GLY	N-CA-C	-5.52	103.28	110.45
1	D	110	VAL	N-CA-C	5.50	115.47	106.72
1	C	258	GLY	N-CA-C	5.50	118.77	110.75
1	D	477	LYS	N-CA-C	-5.49	105.29	111.28
1	B	436	VAL	N-CA-C	5.49	116.63	108.23
1	B	391	TYR	N-CA-C	5.49	114.61	108.25
1	A	391	TYR	N-CA-C	5.48	114.61	108.25
1	B	542	LEU	N-CA-C	-5.47	105.39	111.36
1	D	391	TYR	CA-C-N	-5.47	114.16	119.90
1	D	391	TYR	C-N-CA	-5.47	114.16	119.90
1	D	18	ARG	N-CA-C	-5.46	100.28	109.07
1	C	211	VAL	N-CA-C	-5.44	106.50	111.67
1	A	354	GLN	N-CA-C	-5.43	102.24	110.28
1	A	712	VAL	N-CA-C	5.42	117.11	108.87
1	B	657	GLU	N-CA-C	5.41	119.05	112.23
1	D	557	ILE	N-CA-C	-5.40	107.17	111.81
1	B	486	LYS	N-CA-C	-5.37	104.98	112.45
1	B	548	THR	N-CA-C	-5.36	106.58	113.23
1	C	515	ASP	N-CA-C	5.36	117.20	108.63
1	B	721	ALA	N-CA-C	-5.34	105.37	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	456	CYS	N-CA-C	5.33	117.97	109.81
1	A	380	ILE	CA-C-N	5.26	125.55	119.92
1	A	380	ILE	C-N-CA	5.26	125.55	119.92
1	D	206	GLN	N-CA-C	-5.26	105.02	111.75
2	K	18	DG	C2'-C3'-O3'	-5.26	103.62	111.50
1	C	125	GLU	CA-C-N	5.25	124.75	119.19
1	C	125	GLU	C-N-CA	5.25	124.75	119.19
1	C	150	ASP	N-CA-C	5.24	117.51	109.07
1	A	570	LEU	N-CA-C	5.20	117.62	111.33
1	D	502	ALA	N-CA-C	-5.19	107.61	114.31
1	A	573	VAL	N-CA-C	5.19	118.33	111.17
1	D	755	GLU	N-CA-C	5.18	121.83	110.80
1	C	121	ASP	N-CA-C	5.17	119.75	112.72
1	C	712	VAL	N-CA-C	5.17	116.72	108.87
1	C	331	VAL	CB-CA-C	-5.16	105.28	111.88
1	C	456	CYS	N-CA-C	5.14	117.67	109.81
1	A	449	ARG	CA-C-N	5.13	126.26	119.84
1	A	449	ARG	C-N-CA	5.13	126.26	119.84
1	C	449	ARG	CA-C-N	5.10	126.22	119.84
1	C	449	ARG	C-N-CA	5.10	126.22	119.84
1	C	730	LEU	N-CA-C	-5.07	103.78	110.43
1	D	394	ALA	CA-C-N	-5.06	115.59	122.93
1	D	394	ALA	C-N-CA	-5.06	115.59	122.93
1	C	487	GLY	N-CA-C	-5.06	106.59	113.37
1	D	779	ILE	N-CA-C	-5.05	108.05	112.90
1	A	121	ASP	N-CA-C	5.05	119.12	112.25
1	A	178	VAL	CA-C-N	5.03	126.13	119.84
1	A	178	VAL	C-N-CA	5.03	126.13	119.84
1	C	457	SER	CA-C-N	5.01	126.11	119.84
1	C	457	SER	C-N-CA	5.01	126.11	119.84
1	C	215	GLY	N-CA-C	-5.01	103.88	110.74
1	D	379	VAL	N-CA-C	5.01	115.06	107.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	12	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7284	0	7114	418	0
1	B	7315	0	7162	372	0
1	C	7312	0	7157	531	0
1	D	7165	0	6893	654	0
2	E	265	0	146	17	0
2	G	370	0	205	20	0
2	I	370	0	205	29	0
2	K	370	0	205	23	0
3	F	262	0	149	9	0
3	H	304	0	171	10	0
3	J	304	0	171	17	0
3	L	301	0	162	20	0
4	B	30	0	12	3	0
4	J	30	0	12	2	0
5	A	59	0	0	8	0
5	B	50	0	0	3	0
5	C	40	0	0	6	0
5	D	27	0	0	3	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	3	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	1	0
5	L	1	0	0	0	0
All	All	31870	0	29764	2088	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 34.

All (2088) 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:C:149:PHE:HB3	1:C:197:LEU:HD11	1.20	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:THR:HG23	1:B:733:GLN:HE21	0.98	1.13
1:C:424:ASN:HD22	1:C:677:LYS:HD3	1.01	1.10
1:D:214:THR:HG22	1:D:215:GLY:H	1.10	1.09
3:L:110:DA:H2''	3:L:111:DT:H5'	1.34	1.08
2:E:10:DA:H2''	2:E:11:DC:H5''	1.14	1.07
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.11	1.05
1:D:164:ILE:H	1:D:164:ILE:HD13	1.22	1.05
1:C:511:ASP:HB3	1:C:534:SER:HB2	1.35	1.03
1:A:514:LEU:H	1:A:541:MET:HE2	1.21	1.03
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.39	1.03
3:L:108:DT:H2''	3:L:109:DC:H5''	1.37	1.02
1:A:642:ARG:H	1:A:646:HIS:CD2	1.77	1.02
1:B:465:LYS:HE3	1:B:677:LYS:HA	1.39	1.01
1:A:493:GLN:HB2	1:A:549:GLU:HG3	1.40	1.01
1:B:668:ARG:HH11	1:B:668:ARG:HB2	1.24	1.01
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.42	0.99
1:C:25:ARG:NH2	1:C:27:ARG:HH22	1.60	0.98
2:E:8:DT:H1'	2:E:9:DG:H5''	1.44	0.98
1:D:491:ALA:O	1:D:495:ASN:HB2	1.66	0.96
2:E:10:DA:H2''	2:E:11:DC:C5'	1.95	0.95
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.47	0.95
1:D:606:ASN:HD21	1:D:614:GLU:H	1.04	0.95
1:D:752:MET:HE2	1:D:889:LEU:HD12	1.49	0.94
1:C:25:ARG:HH21	1:C:27:ARG:HH22	1.12	0.94
1:D:517:ASP:HB3	1:D:519:ARG:HG2	1.50	0.94
1:C:512:GLU:HG3	1:C:513:PRO:HD2	1.45	0.94
1:B:732:THR:HG23	1:B:733:GLN:NE2	1.83	0.94
1:B:499:ILE:HG22	1:B:542:LEU:HD22	1.49	0.93
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.67	0.93
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.49	0.93
1:C:392:PRO:O	1:C:587:THR:HG21	1.69	0.92
1:D:300:VAL:HG23	1:D:301:GLY:H	1.34	0.92
1:C:572:ASN:ND2	1:C:574:TRP:H	1.67	0.92
1:A:642:ARG:H	1:A:646:HIS:HD2	0.98	0.92
2:G:15:DC:H42	3:H:103:DG:H1	1.18	0.92
1:D:82:ALA:H	1:D:382:GLN:HE21	0.92	0.92
1:C:424:ASN:ND2	1:C:677:LYS:HD3	1.84	0.92
3:L:108:DT:H2''	3:L:109:DC:C5'	2.00	0.91
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.52	0.91
1:D:395:PHE:HB2	1:D:591:GLN:CD	1.96	0.90
1:A:408:MET:HE1	1:A:659:MET:HE1	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:DG:H2''	3:F:104:DG:H5'	1.52	0.90
1:D:136:ILE:HG23	1:D:149:PHE:HB2	1.53	0.90
1:D:97:TYR:HB3	1:D:101:ILE:HD11	1.51	0.90
1:B:636:VAL:O	1:B:640:LYS:HE2	1.71	0.90
1:D:830:VAL:HG23	1:D:848:TRP:O	1.70	0.90
2:E:10:DA:C2'	2:E:11:DC:H5''	2.02	0.90
1:A:752:MET:HG3	1:A:760:LEU:HD13	1.52	0.90
1:D:449:ARG:NH1	1:D:452:ASP:HB3	1.85	0.89
1:D:133:ILE:HD11	1:D:229:ARG:HG2	1.52	0.89
1:B:668:ARG:HB2	1:B:668:ARG:NH1	1.89	0.88
1:D:15:ILE:HG23	1:D:65:MET:HE1	1.53	0.88
1:C:533:LEU:HD13	1:C:538:LEU:HG	1.53	0.88
1:A:347:MET:HB2	1:A:558:ASN:HD21	1.38	0.88
1:D:347:MET:HG2	1:D:358:VAL:HG13	1.53	0.88
1:D:509:SER:HB3	1:D:534:SER:HB3	1.55	0.88
1:D:443:ILE:HD13	1:D:595:GLN:NE2	1.89	0.87
1:A:516:VAL:HB	1:A:522:PHE:HZ	1.38	0.87
1:D:727:ILE:HG23	1:D:730:LEU:HD12	1.56	0.86
2:I:14:DC:H2''	2:I:15:DC:H5''	1.58	0.86
1:B:732:THR:CG2	1:B:733:GLN:HE21	1.85	0.86
1:D:494:ARG:O	1:D:494:ARG:HG2	1.75	0.86
1:D:751:ARG:NH1	1:D:763:TYR:HB2	1.89	0.85
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.40	0.85
1:D:398:GLU:HB3	1:D:705:LYS:HE3	1.58	0.85
2:I:15:DC:H2''	2:I:16:DG:C8	2.11	0.85
1:D:791:TYR:CE2	1:D:802:PRO:HD3	2.12	0.85
1:B:514:LEU:HG	1:B:541:MET:HE1	1.58	0.85
1:C:541:MET:CE	1:C:542:LEU:HB2	2.07	0.85
1:C:159:VAL:HG11	1:C:317:HIS:HB3	1.58	0.85
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.20	0.84
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.56	0.84
2:G:11:DC:H2''	2:G:12:DA:H5'	1.59	0.84
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.57	0.84
1:D:293:ILE:HD12	1:D:294:SER:N	1.92	0.84
1:A:308:PRO:HG2	1:A:311:LYS:HG3	1.59	0.84
1:B:171:GLN:HE22	1:B:303:LEU:HD13	1.41	0.84
1:D:214:THR:HG22	1:D:215:GLY:N	1.92	0.84
1:D:82:ALA:N	1:D:382:GLN:HE21	1.74	0.84
1:A:703:THR:HG21	1:A:707:ARG:HD3	1.57	0.83
1:D:82:ALA:H	1:D:382:GLN:NE2	1.76	0.83
1:C:502:ALA:HB1	1:C:533:LEU:HD12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLU:HG2	1:D:334:ILE:HG23	1.61	0.83
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.60	0.82
1:C:206:GLN:HA	1:C:206:GLN:HE21	1.42	0.82
1:C:855:THR:HG22	1:C:857:LEU:H	1.43	0.82
1:D:116:GLU:HG2	1:D:324:ASN:HD22	1.45	0.82
1:A:176:ASP:HA	1:A:319:ARG:NH2	1.94	0.82
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.45	0.82
1:C:611:THR:HG22	1:C:612:GLU:H	1.42	0.82
1:A:863:LEU:HA	1:A:866:MET:HE3	1.60	0.82
1:D:224:PRO:HA	1:D:263:ILE:HD12	1.62	0.82
2:E:11:DC:H2''	2:E:12:DA:H5'	1.62	0.82
1:C:818:ASN:ND2	1:C:857:LEU:HD11	1.94	0.81
1:B:408:MET:HE1	1:B:655:ALA:HB2	1.62	0.81
1:C:180:SER:HA	1:C:183:ILE:HD12	1.61	0.81
1:D:791:TYR:CD2	1:D:801:CYS:HA	2.15	0.81
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.62	0.81
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.63	0.81
1:D:514:LEU:HD21	1:D:526:ILE:HG23	1.63	0.81
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.63	0.81
1:C:72:ILE:O	1:C:76:GLU:HG3	1.80	0.81
1:C:133:ILE:HD12	1:C:198:LEU:HD21	1.63	0.81
1:A:514:LEU:HD21	1:A:526:ILE:HG22	1.63	0.80
1:C:541:MET:HE3	1:C:542:LEU:HB2	1.63	0.80
1:D:238:THR:HG23	1:D:241:ARG:HH21	1.45	0.80
1:C:511:ASP:CB	1:C:534:SER:HB2	2.09	0.80
2:I:13:DG:H5''	2:I:13:DG:H8	1.44	0.80
1:A:489:MET:HE1	1:A:553:MET:SD	2.20	0.80
1:A:731:GLU:HG3	1:A:879:PRO:HB3	1.63	0.79
1:D:739:LYS:O	1:D:743:LYS:HG3	1.82	0.79
1:C:491:ALA:HA	1:C:494:ARG:HE	1.47	0.79
1:D:151:LEU:HD12	1:D:153:ASN:O	1.82	0.79
1:A:422:GLN:NE2	1:A:681:MET:HG2	1.95	0.79
1:C:572:ASN:HD22	1:C:574:TRP:H	1.26	0.79
1:A:761:GLN:OE1	1:A:893:LYS:HG2	1.82	0.79
1:D:621:ASP:O	1:D:621:ASP:OD2	2.01	0.79
1:C:254:GLU:HB2	1:C:258:GLY:O	1.83	0.79
1:D:391:TYR:OH	1:D:571:GLY:HA3	1.83	0.79
1:D:734:LYS:HZ3	2:K:7:DA:H4'	1.48	0.78
1:A:279:LYS:C	1:A:280:PHE:HD1	1.92	0.78
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.19	0.78
1:B:686:GLU:OE2	1:B:716:GLU:HG3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:HG2	1:B:599:ARG:HH11	1.47	0.78
1:C:216:TRP:NE1	1:C:274:ILE:HD12	1.98	0.78
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.65	0.78
1:A:642:ARG:N	1:A:646:HIS:HD2	1.80	0.77
1:A:48:LYS:HD3	1:A:377:ASN:CG	2.10	0.77
1:C:159:VAL:HG12	1:C:160:GLU:H	1.49	0.77
1:D:698:ILE:HG12	1:D:752:MET:O	1.85	0.77
1:C:553:MET:HA	1:C:553:MET:HE3	1.65	0.77
1:D:734:LYS:NZ	2:K:7:DA:H4'	1.99	0.77
1:C:495:ASN:ND2	1:C:521:ASP:HA	1.99	0.77
1:D:391:TYR:HE2	1:D:583:ALA:HB1	1.47	0.77
1:A:249:ARG:NH2	1:A:251:LYS:HZ1	1.83	0.77
1:D:395:PHE:HB2	1:D:591:GLN:OE1	1.84	0.77
1:D:4:PHE:HB3	5:D:915:HOH:O	1.84	0.77
1:D:391:TYR:CE2	1:D:583:ALA:HB1	2.19	0.77
1:A:97:TYR:O	1:A:352:LYS:HE2	1.85	0.77
1:C:118:THR:OG1	1:C:313:ARG:HG3	1.85	0.77
1:C:312:LEU:HG	1:C:320:TYR:HD1	1.49	0.77
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.13	0.77
1:D:298:LEU:HB2	1:D:300:VAL:HG22	1.67	0.77
1:A:410:PHE:HB2	1:A:683:MET:HE2	1.66	0.77
1:D:204:PHE:CE1	1:D:208:LYS:HD2	2.20	0.76
1:D:505:ASN:N	1:D:506:PRO:HD3	2.00	0.76
2:I:4:CTG:H2''	2:I:5:DG:H5'	1.67	0.76
1:A:410:PHE:CB	1:A:683:MET:HE2	2.15	0.76
1:D:355:ILE:O	1:D:358:VAL:HG23	1.85	0.76
1:B:511:ASP:OD1	1:B:533:LEU:HA	1.84	0.76
1:D:72:ILE:O	1:D:76:GLU:HG3	1.86	0.76
1:A:516:VAL:HB	1:A:522:PHE:CZ	2.22	0.75
1:A:404:TYR:CD1	1:A:618:LEU:HD22	2.22	0.75
1:C:806:ARG:HG2	1:C:806:ARG:HH11	1.51	0.75
3:L:110:DA:H2''	3:L:111:DT:C5'	2.15	0.75
1:C:34:LYS:HE2	1:C:63:ALA:HA	1.68	0.75
1:D:775:ASN:HD22	1:D:776:TYR:H	1.32	0.75
1:C:300:VAL:HG22	1:C:330:ARG:HH12	1.49	0.75
2:K:16:DG:H2''	2:K:17:DC:H5''	1.68	0.75
1:A:493:GLN:HB2	1:A:549:GLU:CG	2.17	0.75
1:D:273:TYR:OH	1:D:335:ASP:HA	1.86	0.75
3:F:104:DG:H2''	3:F:105:DC:O5'	1.86	0.75
2:K:14:DC:H2''	2:K:15:DC:H5'	1.67	0.75
1:C:120:PRO:O	1:C:819:ILE:HG21	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:HB3	1:D:197:LEU:CD2	2.17	0.74
1:B:669:GLU:O	1:B:672:GLU:HG3	1.87	0.74
1:C:143:ASP:O	1:C:145:ARG:HG2	1.87	0.74
1:C:825:VAL:HB	1:C:828:GLU:CD	2.13	0.74
1:D:441:ASP:HB3	1:D:447:ALA:HB2	1.67	0.74
1:D:440:HIS:CE1	1:D:444:ASN:HD21	2.05	0.74
1:C:424:ASN:HD22	1:C:677:LYS:CD	1.92	0.74
1:D:272:ASP:OD2	1:D:274:ILE:HG22	1.88	0.74
1:D:605:LEU:HD21	1:D:659:MET:HE3	1.70	0.74
1:B:397:LYS:HD3	1:B:619:TYR:HA	1.68	0.73
1:B:514:LEU:HD21	1:B:530:ILE:HG12	1.71	0.73
1:B:749:ILE:O	1:B:753:LEU:HD13	1.88	0.73
1:D:711:ASN:OD1	1:D:723:PRO:HB2	1.89	0.73
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.52	0.73
1:C:302:LYS:HB2	1:C:302:LYS:HZ3	1.52	0.73
1:C:511:ASP:HB3	1:C:534:SER:CB	2.15	0.73
1:C:572:ASN:HD22	1:C:574:TRP:N	1.86	0.73
1:D:686:GLU:OE2	1:D:716:GLU:HG2	1.88	0.73
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.19	0.73
1:B:97:TYR:HB3	1:B:101:ILE:HD11	1.68	0.73
1:D:82:ALA:O	1:D:382:GLN:HG3	1.88	0.73
2:I:3:DT:H2''	2:I:4:CTG:H72	1.71	0.73
1:A:703:THR:CG2	1:A:707:ARG:HD3	2.19	0.72
1:C:507:ASN:HB3	1:C:532:LYS:HA	1.72	0.72
2:I:14:DC:H2''	2:I:15:DC:C5'	2.18	0.72
1:D:163:SER:HB2	1:D:165:GLU:OE2	1.90	0.72
1:A:406:TYR:HB3	1:A:629:ALA:HB3	1.71	0.72
1:D:398:GLU:HB3	1:D:705:LYS:CE	2.19	0.72
1:C:900:MET:HA	1:C:900:MET:HE3	1.71	0.72
1:D:725:LEU:H	1:D:725:LEU:HD12	1.53	0.72
3:L:108:DT:C2'	3:L:109:DC:H5''	2.15	0.72
1:A:825:VAL:HG22	1:A:828:GLU:HG2	1.72	0.72
1:D:33:TYR:HB3	1:D:65:MET:HE2	1.70	0.72
1:C:534:SER:O	1:C:538:LEU:HB2	1.88	0.71
2:E:11:DC:H2''	2:E:12:DA:C5'	2.18	0.71
1:C:159:VAL:HG11	1:C:317:HIS:CB	2.19	0.71
1:D:238:THR:HG23	1:D:241:ARG:NH2	2.05	0.71
1:A:496:GLY:HA2	1:A:499:ILE:HD12	1.72	0.71
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.55	0.71
1:D:164:ILE:H	1:D:164:ILE:CD1	1.99	0.71
1:D:442:TYR:HB3	1:D:592:MET:CE	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:DC:N4	3:H:103:DG:H1	1.88	0.71
1:B:152:LEU:HD11	1:B:190:PRO:HB2	1.70	0.71
1:C:872:LEU:HD12	1:C:876:PHE:HB3	1.72	0.71
1:B:863:LEU:HA	1:B:866:MET:HE3	1.73	0.71
1:D:770:GLU:O	1:D:774:LEU:HG	1.91	0.71
1:A:163:SER:OG	1:A:166:ILE:HD13	1.91	0.71
1:B:163:SER:H	1:B:318:GLN:HE22	1.37	0.71
1:D:648:VAL:HG12	1:D:719:ARG:HH21	1.55	0.70
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.25	0.70
1:B:776:TYR:HB2	1:B:866:MET:HE1	1.74	0.70
1:C:451:SER:OG	1:C:453:VAL:HG22	1.90	0.70
1:D:212:ILE:HD11	1:D:345:LEU:HD21	1.73	0.70
1:D:685:ARG:HH11	1:D:688:ILE:HG13	1.56	0.70
2:I:14:DC:C2'	2:I:15:DC:H5''	2.20	0.70
1:B:526:ILE:O	1:B:530:ILE:HG13	1.91	0.70
1:D:514:LEU:HB2	1:D:533:LEU:HD11	1.73	0.70
1:D:449:ARG:HH12	1:D:452:ASP:HB3	1.56	0.70
1:B:495:ASN:OD1	1:B:521:ASP:HA	1.91	0.70
1:B:636:VAL:HG13	1:B:640:LYS:HE3	1.73	0.70
1:C:482:ARG:HH12	1:C:560:LYS:HB2	1.56	0.70
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.73	0.70
1:C:78:ILE:HG13	1:C:80:LEU:HD23	1.73	0.70
1:D:399:PRO:O	1:D:401:PRO:HD3	1.91	0.70
1:D:696:LYS:O	1:D:756:GLY:HA2	1.92	0.70
1:C:162:TRP:HB3	1:C:188:TYR:CE1	2.26	0.70
1:C:509:SER:HB3	1:C:532:LYS:HD2	1.73	0.70
1:D:430:ILE:H	1:D:430:ILE:HD12	1.57	0.70
1:B:253:ILE:HD13	1:B:254:GLU:H	1.57	0.69
1:C:538:LEU:O	1:C:538:LEU:HD23	1.89	0.69
1:C:482:ARG:NH1	1:C:560:LYS:HB2	2.07	0.69
1:A:514:LEU:N	1:A:541:MET:HE2	2.01	0.69
1:C:499:ILE:HG13	1:C:541:MET:SD	2.32	0.69
1:D:109:ARG:HE	1:D:208:LYS:HB3	1.57	0.69
2:G:11:DC:H2''	2:G:12:DA:C5'	2.22	0.69
1:D:727:ILE:O	1:D:728:MET:HE2	1.92	0.69
1:D:809:LEU:HA	1:D:812:ASN:HD22	1.57	0.69
1:C:159:VAL:HG12	1:C:160:GLU:N	2.06	0.69
1:D:398:GLU:HA	1:D:705:LYS:HZ2	1.56	0.69
1:A:397:LYS:HB3	1:A:620:GLY:H	1.58	0.69
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.28	0.69
1:C:255:ASN:CG	1:C:256:MET:H	1.98	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ARG:HA	1:A:809:LEU:HD12	1.73	0.69
1:B:523:SER:H	1:B:526:ILE:HD12	1.57	0.69
1:C:104:ASP:OD2	1:C:107:LYS:HG2	1.92	0.69
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.58	0.69
1:C:431:ALA:HA	1:C:464:TYR:CE1	2.28	0.69
1:C:191:PHE:CD1	1:C:197:LEU:HD13	2.28	0.68
1:D:775:ASN:HD22	1:D:776:TYR:N	1.91	0.68
1:D:433:THR:O	1:D:462:MET:HE2	1.94	0.68
1:B:491:ALA:HA	1:B:494:ARG:NH2	2.09	0.68
1:C:199:MET:HG2	1:C:234:PHE:CZ	2.28	0.68
1:D:214:THR:HG21	1:D:273:TYR:HD2	1.59	0.68
1:A:207:GLN:HA	1:A:207:GLN:HE21	1.58	0.68
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.76	0.68
1:B:608:VAL:HG13	1:D:897:LEU:HD13	1.73	0.68
1:B:752:MET:HE3	1:B:889:LEU:HD12	1.75	0.68
1:D:757:GLU:O	1:D:761:GLN:HG3	1.93	0.68
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.74	0.68
1:B:365:TRP:O	1:B:369:ILE:HD12	1.93	0.68
1:A:347:MET:HE3	1:A:364:THR:HG21	1.74	0.68
1:C:179:PRO:O	1:C:183:ILE:HG13	1.94	0.68
1:A:642:ARG:HB2	1:A:642:ARG:NH1	2.09	0.67
1:C:525:GLU:H	1:C:525:GLU:CD	2.00	0.67
1:C:727:ILE:HD13	1:C:749:ILE:HD12	1.75	0.67
1:C:14:SER:HB3	1:C:32:GLU:OE2	1.93	0.67
1:C:322:SER:O	1:C:326:ILE:HG13	1.94	0.67
1:C:490:LEU:O	1:C:494:ARG:HG3	1.93	0.67
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.24	0.67
1:D:493:GLN:HG3	1:D:549:GLU:OE2	1.93	0.67
1:B:303:LEU:HD13	1:B:319:ARG:NH2	2.09	0.67
1:C:542:LEU:C	1:C:546:GLN:HE21	2.02	0.67
1:D:153:ASN:HA	1:D:158:ASN:ND2	2.10	0.67
2:K:11:DC:H4'	2:K:11:DC:OP1	1.93	0.67
1:C:171:GLN:HG2	1:C:177:GLU:OE1	1.95	0.67
2:G:12:DA:H2''	2:G:13:DG:C8	2.30	0.67
2:I:13:DG:H2'	2:I:14:DC:C6	2.30	0.67
1:A:493:GLN:CB	1:A:549:GLU:HG3	2.22	0.67
1:B:503:LEU:HB2	1:B:542:LEU:HD21	1.77	0.67
1:B:597:ILE:HD13	1:B:683:MET:SD	2.35	0.67
1:C:491:ALA:HA	1:C:494:ARG:NE	2.09	0.67
1:A:280:PHE:HE2	1:A:343:LEU:HD22	1.60	0.67
1:B:303:LEU:HD13	1:B:319:ARG:HH22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:O	1:B:420:ILE:HG13	1.94	0.67
1:B:559:ARG:O	1:B:563:ILE:HD12	1.94	0.67
1:C:711:ASN:HD21	1:C:754:GLN:NE2	1.93	0.67
1:D:167:ALA:HA	1:D:176:ASP:HB2	1.77	0.67
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.29	0.67
1:C:523:SER:HB3	1:C:525:GLU:HG2	1.76	0.67
1:D:412:LEU:HG	1:D:623:ASP:O	1.95	0.67
1:A:171:GLN:NE2	1:A:319:ARG:HH12	1.92	0.66
1:A:597:ILE:O	1:A:601:VAL:HG23	1.95	0.66
1:B:642:ARG:HD3	1:B:646:HIS:CE1	2.30	0.66
1:C:432:GLY:C	1:C:462:MET:HE2	2.20	0.66
1:C:109:ARG:NH1	1:C:142:ILE:HD12	2.11	0.66
1:D:458:PRO:HD3	1:D:674:MET:HE2	1.77	0.66
2:I:13:DG:H5''	2:I:13:DG:C8	2.29	0.66
1:A:19:TYR:HE1	1:A:29:ARG:HG2	1.61	0.66
1:A:202:LEU:O	1:A:206:GLN:HG2	1.94	0.66
1:C:505:ASN:N	1:C:506:PRO:HD3	2.11	0.66
1:D:197:LEU:O	1:D:197:LEU:HD13	1.94	0.66
1:A:369:ILE:HG12	1:A:474:GLU:HG3	1.78	0.66
1:C:177:GLU:HG3	1:C:303:LEU:HD11	1.76	0.66
1:C:507:ASN:ND2	1:C:508:LEU:H	1.93	0.66
1:D:777:ILE:HD12	1:D:778:SER:N	2.11	0.66
2:G:10:DA:H2''	2:G:11:DC:C5'	2.26	0.66
1:A:411:ASP:OD2	1:A:686:GLU:HG3	1.95	0.66
1:B:270:VAL:C	1:B:271:LEU:HD12	2.20	0.66
1:D:416:TYR:CD1	1:D:586:ILE:HG22	2.30	0.66
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.77	0.66
2:K:13:DG:H2''	2:K:14:DC:OP2	1.94	0.66
1:A:752:MET:CG	1:A:760:LEU:HD13	2.26	0.66
1:B:449:ARG:HH12	1:B:452:ASP:HB2	1.61	0.66
1:A:722:GLU:HA	1:A:722:GLU:OE2	1.96	0.65
1:D:140:ASP:OD1	1:D:142:ILE:HG12	1.94	0.65
1:B:408:MET:HE1	1:B:655:ALA:CB	2.26	0.65
1:C:808:ILE:HD12	1:C:824:VAL:HG11	1.77	0.65
1:A:495:ASN:C	1:A:497:GLU:H	2.05	0.65
1:B:110:VAL:H	1:B:141:SER:HB3	1.61	0.65
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.79	0.65
1:C:412:LEU:HG	1:C:683:MET:HE3	1.79	0.65
3:F:103:DG:H2''	3:F:104:DG:C5'	2.25	0.65
1:C:509:SER:OG	1:C:532:LYS:HB3	1.97	0.65
1:D:855:THR:HG22	1:D:857:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:O	1:A:48:LYS:HG2	1.95	0.65
1:A:602:ASN:ND2	1:A:616:PHE:H	1.94	0.65
1:C:611:THR:HG22	1:C:612:GLU:N	2.11	0.65
1:D:300:VAL:HG23	1:D:301:GLY:N	2.07	0.65
1:C:272:ASP:CG	1:C:274:ILE:HG22	2.22	0.65
1:C:444:ASN:HA	1:C:599:ARG:HE	1.62	0.65
1:D:503:LEU:HD23	1:D:503:LEU:O	1.97	0.65
1:B:642:ARG:NH1	1:B:646:HIS:ND1	2.41	0.65
1:D:15:ILE:HG13	1:D:31:VAL:HG22	1.79	0.65
1:A:475:ILE:CD1	1:A:566:LEU:HD22	2.27	0.65
1:A:712:VAL:HG22	1:A:724:LYS:O	1.96	0.65
1:D:226:VAL:O	1:D:230:ILE:HG13	1.97	0.65
1:B:272:ASP:CG	1:B:274:ILE:HG22	2.21	0.64
2:E:8:DT:H1'	2:E:9:DG:C5'	2.24	0.64
1:A:499:ILE:HD13	1:A:541:MET:O	1.97	0.64
1:A:171:GLN:HE22	1:A:319:ARG:HH12	1.43	0.64
1:B:478:VAL:O	1:B:559:ARG:HG3	1.97	0.64
1:D:808:ILE:HG23	1:D:824:VAL:HG21	1.78	0.64
1:A:171:GLN:HE22	1:A:319:ARG:HH22	1.43	0.64
1:C:311:LYS:HA	1:C:314:GLU:OE1	1.98	0.64
1:D:112:ASN:HD21	1:D:331:VAL:HG11	1.63	0.64
1:D:507:ASN:O	1:D:509:SER:N	2.30	0.64
1:D:656:ARG:HB3	1:D:656:ARG:HH11	1.61	0.64
1:D:830:VAL:HG23	1:D:848:TRP:C	2.22	0.64
1:C:434:PHE:CE1	1:C:460:GLY:HA2	2.31	0.64
1:C:475:ILE:HG23	1:C:476:THR:N	2.12	0.64
1:D:606:ASN:HD21	1:D:614:GLU:N	1.88	0.64
1:D:727:ILE:CG2	1:D:730:LEU:HD12	2.27	0.64
3:L:111:DT:H2''	3:L:112:DT:H5''	1.79	0.64
1:B:468:ASP:OD1	1:B:677:LYS:HE3	1.98	0.64
1:D:499:ILE:HD13	1:D:541:MET:O	1.95	0.64
1:D:660:GLU:HA	1:D:660:GLU:OE1	1.97	0.64
1:B:303:LEU:HB3	1:B:319:ARG:HH21	1.61	0.64
1:C:251:LYS:HG2	1:C:253:ILE:HG23	1.80	0.64
3:H:110:DA:H2''	3:H:111:DT:H5'	1.80	0.64
1:B:326:ILE:O	1:B:330:ARG:HG2	1.97	0.64
1:C:533:LEU:HB3	1:C:538:LEU:HD12	1.80	0.64
3:J:105:DC:H2''	3:J:106:DT:O5'	1.98	0.64
1:B:536:LYS:HA	1:B:539:ASN:HD22	1.63	0.64
1:C:492:ALA:HB3	5:C:940:HOH:O	1.97	0.64
1:D:143:ASP:O	1:D:145:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:ILE:HA	1:D:529:LYS:HB2	1.79	0.64
1:A:410:PHE:HB2	1:A:683:MET:CE	2.27	0.63
1:D:3:GLU:HG3	1:D:21:ASP:HA	1.79	0.63
1:D:825:VAL:CG2	1:D:828:GLU:HB2	2.28	0.63
1:D:826:GLU:OE1	1:D:826:GLU:N	2.31	0.63
1:A:128:GLN:HB3	1:A:130:LYS:HE3	1.80	0.63
1:A:343:LEU:HD23	1:A:343:LEU:O	1.99	0.63
1:A:403:ARG:HD2	1:A:887:ALA:O	1.99	0.63
1:B:269:SER:HA	1:B:356:GLN:NE2	2.14	0.63
1:D:159:VAL:HG11	1:D:317:HIS:HB2	1.80	0.63
1:A:649:ASP:CG	1:A:719:ARG:HH12	2.05	0.63
1:B:416:TYR:CD2	4:B:907:DTP:H2'1	2.33	0.63
1:D:752:MET:HE1	1:D:884:THR:HA	1.80	0.63
1:B:119:SER:CB	1:B:124:PRO:HG3	2.28	0.63
1:B:439:LEU:O	1:B:443:ILE:HG13	1.98	0.63
1:B:503:LEU:HD12	1:B:542:LEU:HG	1.79	0.63
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.81	0.63
1:D:112:ASN:HD21	1:D:331:VAL:CG1	2.11	0.63
1:D:398:GLU:CA	1:D:705:LYS:HZ2	2.11	0.63
1:B:685:ARG:HG2	5:B:919:HOH:O	1.98	0.63
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.14	0.63
1:C:343:LEU:HG	1:C:558:ASN:HD21	1.64	0.63
1:C:533:LEU:HB3	1:C:538:LEU:CD1	2.28	0.63
1:D:198:LEU:C	1:D:200:GLU:H	2.07	0.63
1:A:308:PRO:HG2	1:A:311:LYS:CG	2.27	0.63
1:C:109:ARG:CZ	1:C:142:ILE:HD12	2.29	0.63
1:C:312:LEU:HG	1:C:320:TYR:CD1	2.33	0.63
1:C:485:HIS:HA	1:C:488:TYR:HB2	1.81	0.63
1:C:505:ASN:N	1:C:506:PRO:CD	2.62	0.63
1:D:256:MET:HE1	2:K:5:DG:N7	2.14	0.63
1:D:606:ASN:ND2	1:D:614:GLU:H	1.88	0.63
1:D:832:VAL:HG22	1:D:847:ALA:HB2	1.81	0.63
1:A:319:ARG:HD3	5:A:907:HOH:O	1.99	0.63
1:B:66:ARG:HB3	5:B:911:HOH:O	1.98	0.63
1:D:204:PHE:HE1	1:D:208:LYS:HD2	1.63	0.63
1:D:791:TYR:HD2	1:D:801:CYS:HA	1.64	0.63
1:A:503:LEU:HA	1:A:538:LEU:HD13	1.80	0.62
1:B:313:ARG:HG2	1:B:313:ARG:NH1	2.12	0.62
1:B:329:TYR:O	1:B:333:GLN:HG3	1.99	0.62
1:C:314:GLU:H	1:C:314:GLU:CD	2.07	0.62
1:C:434:PHE:CE2	1:C:450:PRO:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:C	1:A:64:ASN:HD22	2.06	0.62
1:A:422:GLN:NE2	1:A:681:MET:HE3	2.14	0.62
1:A:597:ILE:HD11	1:A:663:ILE:HG23	1.80	0.62
1:B:534:SER:O	1:B:538:LEU:HB2	1.99	0.62
1:D:136:ILE:HD11	1:D:201:TYR:CE1	2.34	0.62
1:A:280:PHE:HD2	1:A:343:LEU:HD13	1.63	0.62
1:C:25:ARG:NH2	1:C:27:ARG:NH2	2.43	0.62
1:C:144:ASP:O	1:C:145:ARG:HD3	1.99	0.62
1:C:592:MET:HE3	1:C:670:MET:SD	2.39	0.62
1:D:217:ASN:OD1	1:D:220:SER:HB2	1.99	0.62
1:D:523:SER:C	1:D:527:LYS:HG3	2.25	0.62
1:D:658:ARG:HG3	1:D:658:ARG:HH11	1.64	0.62
2:K:10:DA:H2''	2:K:11:DC:O5'	1.99	0.62
1:C:163:SER:OG	1:C:166:ILE:HG13	2.00	0.62
1:A:747:GLU:OE2	1:A:747:GLU:HA	1.99	0.62
2:K:13:DG:H1	3:L:105:DC:H42	1.47	0.62
1:B:305:TYR:CD2	1:B:312:LEU:HD22	2.35	0.62
1:C:188:TYR:CD2	1:C:190:PRO:HD3	2.34	0.62
1:C:193:ASN:OD1	1:C:196:GLU:HG2	2.00	0.62
1:A:74:ARG:O	1:A:77:ASP:HB2	2.00	0.62
1:A:412:LEU:HG	1:A:683:MET:HG3	1.80	0.62
1:A:836:ARG:HG3	1:A:836:ARG:HH11	1.64	0.62
1:B:668:ARG:HH11	1:B:668:ARG:CB	2.08	0.62
1:C:254:GLU:CB	1:C:259:SER:HA	2.29	0.62
1:C:481:GLN:HB3	1:C:559:ARG:HH11	1.63	0.62
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.35	0.62
1:C:477:LYS:O	1:C:481:GLN:HG3	1.99	0.62
1:C:854:ILE:HG22	1:C:859:LYS:HD3	1.82	0.62
1:A:500:LYS:HA	1:A:503:LEU:HD12	1.82	0.61
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.33	0.61
1:D:145:ARG:HD3	1:D:185:LYS:O	2.00	0.61
1:C:477:LYS:HG2	1:C:481:GLN:HE21	1.63	0.61
1:D:339:GLN:HG2	1:D:342:ASN:HB3	1.80	0.61
1:D:855:THR:CG2	1:D:857:LEU:HG	2.30	0.61
1:C:402:ASN:ND2	1:C:403:ARG:H	1.98	0.61
1:D:323:TYR:O	1:D:326:ILE:HG13	1.99	0.61
1:D:733:GLN:HA	1:D:733:GLN:NE2	2.13	0.61
1:A:475:ILE:HD11	1:A:566:LEU:HD22	1.82	0.61
1:A:602:ASN:HD21	1:A:617:VAL:H	1.46	0.61
1:A:705:LYS:HB2	2:E:8:DT:OP1	2.00	0.61
1:B:231:LYS:HD2	1:B:236:GLU:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ASN:HD21	1:B:521:ASP:HA	1.64	0.61
1:D:165:GLU:H	1:D:165:GLU:CD	2.07	0.61
1:D:206:GLN:NE2	1:D:241:ARG:O	2.34	0.61
1:A:19:TYR:CE1	1:A:29:ARG:HG2	2.35	0.61
1:B:495:ASN:ND2	1:B:521:ASP:HA	2.16	0.61
1:C:431:ALA:HA	1:C:464:TYR:HE1	1.65	0.61
1:D:402:ASN:CG	1:D:403:ARG:H	2.08	0.61
1:D:614:GLU:HB3	1:D:616:PHE:HE2	1.66	0.61
1:C:128:GLN:HB3	5:C:942:HOH:O	2.01	0.61
1:D:804:HIS:O	1:D:808:ILE:HG13	2.01	0.61
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.61
1:C:49:TYR:CE1	1:C:59:ARG:HB2	2.36	0.61
1:D:621:ASP:O	1:D:623:ASP:N	2.30	0.61
1:D:818:ASN:C	1:D:820:ASP:H	2.09	0.61
1:A:415:LEU:O	1:A:419:ILE:HG13	2.01	0.61
1:A:642:ARG:N	1:A:646:HIS:CD2	2.59	0.61
1:B:176:ASP:O	1:B:303:LEU:HD12	2.01	0.61
1:C:59:ARG:HG3	1:C:59:ARG:HH11	1.65	0.61
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.83	0.61
1:D:152:LEU:HD11	1:D:190:PRO:HB2	1.83	0.61
1:C:41:CYS:CB	1:C:58:THR:HG22	2.28	0.61
1:A:422:GLN:HG3	1:A:678:GLN:O	2.00	0.60
1:D:412:LEU:CD1	1:D:623:ASP:HA	2.27	0.60
1:B:34:LYS:HZ2	1:B:61:LEU:HD11	1.66	0.60
1:C:36:SER:HB3	1:C:59:ARG:CD	2.31	0.60
1:D:51:ASP:OD1	1:D:53:TYR:N	2.29	0.60
1:D:119:SER:HB2	1:D:131:HIS:CD2	2.36	0.60
1:D:381:PRO:HG2	1:D:576:ARG:HG2	1.82	0.60
1:D:402:ASN:CG	1:D:403:ARG:N	2.57	0.60
1:D:499:ILE:O	1:D:503:LEU:HB2	1.99	0.60
3:H:110:DA:H2''	3:H:111:DT:C5'	2.32	0.60
2:K:16:DG:H2''	2:K:17:DC:C5'	2.32	0.60
1:C:738:PRO:HG2	1:C:741:VAL:HB	1.84	0.60
1:C:797:PRO:HG3	1:C:806:ARG:HE	1.67	0.60
1:D:146:PHE:CE2	1:D:182:ILE:HG13	2.36	0.60
1:A:64:ASN:HD21	1:A:67:ASP:CG	2.09	0.60
1:B:618:LEU:HD11	1:B:702:TRP:CZ3	2.36	0.60
1:C:164:ILE:HD11	1:C:183:ILE:O	2.01	0.60
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.36	0.60
1:D:416:TYR:HD1	1:D:586:ILE:HG22	1.65	0.60
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:O	1:A:591:GLN:HB2	2.02	0.60
1:A:802:PRO:CG	3:F:109:DC:H4'	2.31	0.60
1:B:465:LYS:HE3	1:B:677:LYS:CA	2.23	0.60
1:D:863:LEU:HA	1:D:866:MET:HE2	1.84	0.60
1:D:214:THR:CG2	1:D:215:GLY:H	1.92	0.60
1:D:599:ARG:HB3	1:D:599:ARG:HH11	1.66	0.60
1:D:648:VAL:HG12	1:D:719:ARG:NH2	2.15	0.60
1:A:738:PRO:HG2	1:A:741:VAL:HB	1.84	0.60
1:A:758:GLU:O	1:A:762:GLU:HG3	2.01	0.60
1:C:34:LYS:HB3	1:C:61:LEU:HD21	1.84	0.60
1:C:324:ASN:HD22	1:C:324:ASN:C	2.08	0.60
1:C:858:ILE:O	1:C:862:VAL:HG23	2.02	0.60
1:D:249:ARG:HB3	1:D:264:THR:OG1	2.02	0.60
1:D:356:GLN:OE1	1:D:356:GLN:N	2.26	0.60
1:A:508:LEU:HD22	1:A:508:LEU:N	2.17	0.60
1:A:745:LEU:HD13	1:A:876:PHE:CE1	2.37	0.60
1:B:511:ASP:OD2	1:B:533:LEU:HD23	2.01	0.60
1:B:533:LEU:HD23	1:B:534:SER:H	1.66	0.60
1:D:198:LEU:HD22	1:D:198:LEU:N	2.16	0.60
1:D:395:PHE:HB2	1:D:591:GLN:NE2	2.16	0.60
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.31	0.59
1:A:505:ASN:N	1:A:506:PRO:HD3	2.16	0.59
1:C:300:VAL:CG2	1:C:330:ARG:HH12	2.15	0.59
1:C:412:LEU:CD1	1:C:415:LEU:HD13	2.31	0.59
1:D:277:TYR:O	1:D:281:SER:CB	2.50	0.59
1:D:403:ARG:HH22	1:D:889:LEU:HD21	1.67	0.59
1:A:176:ASP:O	1:A:303:LEU:HD21	2.02	0.59
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.83	0.59
1:B:362:ILE:HG12	2:G:2:DG:OP2	2.02	0.59
1:B:660:GLU:HB3	1:B:661:PRO:HD3	1.83	0.59
1:C:795:GLY:O	1:C:813:ARG:HD3	2.02	0.59
1:D:734:LYS:HG3	1:D:736:SER:H	1.67	0.59
3:J:113:DC:H5'	3:J:113:DC:H6	1.67	0.59
1:D:430:ILE:HD12	1:D:430:ILE:N	2.17	0.59
1:D:792:ASP:OD1	1:D:795:GLY:HA2	2.02	0.59
1:B:262:ILE:HG13	1:B:262:ILE:O	2.01	0.59
1:D:109:ARG:NH1	1:D:142:ILE:HD11	2.17	0.59
1:A:874:LYS:HE2	2:E:11:DC:OP1	2.02	0.59
1:D:733:GLN:HA	1:D:733:GLN:HE21	1.67	0.59
1:D:806:ARG:NH1	1:D:806:ARG:HB3	2.16	0.59
1:A:49:TYR:CE1	1:A:59:ARG:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:VAL:HG12	1:B:263:ILE:HD13	1.84	0.59
1:B:410:PHE:HZ	1:B:659:MET:HE3	1.67	0.59
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.85	0.59
1:D:534:SER:O	1:D:538:LEU:HG	2.03	0.59
1:C:898:PHE:CD2	1:C:898:PHE:N	2.67	0.59
2:E:8:DT:H2"	2:E:9:DG:OP2	2.02	0.59
2:I:9:DG:H2"	2:I:10:DA:H5'	1.84	0.59
1:C:3:GLU:HB2	1:C:20:ILE:O	2.02	0.59
1:B:538:LEU:HD22	1:B:542:LEU:HD23	1.84	0.59
1:C:176:ASP:O	1:C:177:GLU:HB2	2.02	0.59
1:D:191:PHE:CD2	1:D:197:LEU:HA	2.37	0.59
1:D:642:ARG:HH21	1:D:646:HIS:CD2	2.21	0.59
1:B:221:PHE:C	1:B:224:PRO:HD2	2.28	0.59
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.83	0.58
1:B:528:GLU:HA	1:B:531:LYS:HD2	1.85	0.58
1:C:898:PHE:H	1:C:898:PHE:HD2	1.50	0.58
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.03	0.58
1:B:354:GLN:HB3	1:B:356:GLN:OE1	2.02	0.58
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.02	0.58
1:C:270:VAL:O	1:C:271:LEU:HD23	2.02	0.58
1:C:491:ALA:O	1:C:493:GLN:N	2.36	0.58
1:C:557:ILE:O	1:C:561:LEU:HD13	2.02	0.58
1:C:793:VAL:HG12	1:C:793:VAL:O	2.03	0.58
1:D:85:MET:HA	1:D:380:ILE:HD11	1.85	0.58
1:D:656:ARG:HB3	1:D:656:ARG:NH1	2.16	0.58
1:D:775:ASN:ND2	1:D:776:TYR:H	2.00	0.58
2:G:16:DG:H1'	2:G:17:DC:H5"	1.84	0.58
1:A:37:LEU:HD11	1:A:72:ILE:HD11	1.84	0.58
1:B:34:LYS:NZ	1:B:61:LEU:HD11	2.19	0.58
1:B:101:ILE:HG21	1:B:349:TYR:HB3	1.85	0.58
3:J:103:DG:H2"	3:J:104:DG:OP2	2.03	0.58
1:D:696:LYS:CB	1:D:756:GLY:HA3	2.34	0.58
1:A:236:GLU:O	1:A:240:LYS:HG2	2.03	0.58
1:A:414:SER:O	1:A:417:PRO:HD2	2.03	0.58
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.84	0.58
1:B:514:LEU:CG	1:B:541:MET:HE1	2.29	0.58
1:D:345:LEU:HA	1:D:355:ILE:HD12	1.85	0.58
1:D:686:GLU:OE2	1:D:686:GLU:HA	2.03	0.58
1:B:164:ILE:HD13	1:B:164:ILE:N	2.19	0.58
1:B:495:ASN:CG	1:B:521:ASP:HA	2.29	0.58
1:C:18:ARG:NH2	1:C:209:THR:HG22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:ND2	1:C:256:MET:H	2.01	0.58
1:C:518:TYR:HB2	1:C:548:THR:HG21	1.85	0.58
1:C:572:ASN:ND2	1:C:574:TRP:N	2.42	0.58
1:D:432:GLY:O	1:D:461:MET:HE3	2.04	0.58
1:D:660:GLU:HB3	1:D:661:PRO:HD3	1.85	0.58
2:K:16:DG:C2'	2:K:17:DC:H5''	2.34	0.58
1:B:380:ILE:HD12	1:B:576:ARG:CZ	2.34	0.58
1:D:398:GLU:CB	1:D:705:LYS:HZ2	2.15	0.58
1:D:405:LYS:O	1:D:690:GLY:HA2	2.03	0.58
1:A:280:PHE:HD1	1:A:280:PHE:N	2.01	0.58
1:A:280:PHE:N	1:A:280:PHE:CD1	2.72	0.58
1:A:653:LYS:HE3	1:A:657:GLU:OE1	2.03	0.58
1:B:101:ILE:HG21	1:B:349:TYR:CD1	2.39	0.58
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.39	0.58
1:C:461:MET:SD	1:C:581:ARG:HB3	2.43	0.58
1:D:150:ASP:OD2	1:D:321:ILE:HG13	2.04	0.58
1:D:362:ILE:HG22	1:D:363:LYS:N	2.19	0.58
1:A:250:VAL:HG23	1:A:250:VAL:O	2.02	0.58
1:B:71:TRP:CZ2	1:B:75:MET:HE2	2.39	0.58
1:C:254:GLU:HB3	1:C:259:SER:HA	1.85	0.58
1:D:81:GLU:HG3	1:D:382:GLN:HB2	1.86	0.58
1:D:458:PRO:HG2	1:D:592:MET:SD	2.44	0.58
1:D:321:ILE:O	1:D:325:ILE:HG13	2.04	0.58
1:D:775:ASN:ND2	1:D:776:TYR:N	2.52	0.58
1:A:105:HIS:HD2	1:A:106:THR:N	2.01	0.57
1:B:405:LYS:O	1:B:690:GLY:HA2	2.04	0.57
1:B:461:MET:SD	1:B:581:ARG:HG2	2.43	0.57
1:C:136:ILE:HB	1:C:149:PHE:HB2	1.86	0.57
1:C:489:MET:HG2	1:C:493:GLN:HE21	1.68	0.57
1:D:256:MET:N	2:K:4:CTG:OP2	2.36	0.57
1:A:64:ASN:ND2	1:A:67:ASP:H	2.02	0.57
1:A:387:PRO:O	1:A:389:GLN:HG3	2.04	0.57
1:C:143:ASP:OD1	1:C:208:LYS:NZ	2.37	0.57
1:D:154:SER:C	1:D:156:TYR:H	2.12	0.57
1:D:198:LEU:O	1:D:200:GLU:N	2.38	0.57
1:A:872:LEU:HD12	1:A:876:PHE:HB3	1.85	0.57
1:B:795:GLY:O	1:B:813:ARG:HD3	2.04	0.57
1:C:206:GLN:HE21	1:C:206:GLN:CA	2.15	0.57
1:C:361:PRO:HD2	2:I:2:DG:OP2	2.03	0.57
1:C:512:GLU:CG	1:C:513:PRO:HD2	2.27	0.57
1:C:611:THR:HG21	1:C:614:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:CYS:SG	1:D:806:ARG:HG2	2.45	0.57
2:G:10:DA:H2''	2:G:11:DC:H5''	1.85	0.57
1:A:835:LEU:HD11	1:A:846:ILE:HB	1.86	0.57
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.87	0.57
1:D:765:LYS:O	1:D:768:GLU:HB2	2.03	0.57
1:D:830:VAL:HA	1:D:850:SER:HB2	1.87	0.57
2:I:16:DG:H5'	5:I:118:HOH:O	2.04	0.57
1:A:41:CYS:SG	1:A:58:THR:HG23	2.43	0.57
1:A:81:GLU:OE2	1:A:83:LEU:HG	2.05	0.57
1:C:422:GLN:HG3	1:C:678:GLN:O	2.05	0.57
1:D:240:LYS:O	1:D:246:ARG:HA	2.04	0.57
1:D:848:TRP:N	1:D:848:TRP:CD1	2.73	0.57
2:K:11:DC:H2''	2:K:12:DA:H8	1.68	0.57
1:A:48:LYS:HD3	1:A:377:ASN:OD1	2.04	0.57
1:A:112:ASN:HB2	5:A:947:HOH:O	2.04	0.57
1:B:576:ARG:HG3	1:B:576:ARG:O	2.04	0.57
1:C:172:GLU:H	1:C:172:GLU:CD	2.11	0.57
1:A:802:PRO:HG2	3:F:109:DC:H4'	1.85	0.57
1:A:870:VAL:O	1:A:874:LYS:HG2	2.04	0.57
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.39	0.57
1:C:163:SER:HB3	1:C:166:ILE:HD12	1.85	0.57
1:C:416:TYR:HB2	1:C:417:PRO:HD3	1.87	0.57
1:D:159:VAL:HG21	1:D:317:HIS:ND1	2.20	0.57
2:E:9:DG:H2''	2:E:10:DA:OP2	2.03	0.57
3:F:112:DT:H2''	3:F:113:DC:C6	2.39	0.57
1:A:426:SER:OG	1:A:427:PRO:HD2	2.05	0.57
1:B:668:ARG:O	1:B:672:GLU:HG2	2.05	0.57
1:B:685:ARG:NH2	1:B:714:ASP:OD2	2.31	0.57
1:C:37:LEU:C	1:C:38:PHE:CD1	2.83	0.57
1:D:883:PHE:CD2	1:D:883:PHE:N	2.71	0.57
1:A:41:CYS:HB3	1:A:58:THR:HG23	1.87	0.57
1:C:512:GLU:HG3	1:C:513:PRO:CD	2.28	0.57
1:D:330:ARG:O	1:D:334:ILE:HG13	2.05	0.57
1:D:503:LEU:HD11	1:D:539:ASN:OD1	2.04	0.57
1:D:751:ARG:HD3	1:D:759:SER:OG	2.04	0.57
1:A:83:LEU:N	1:A:83:LEU:HD12	2.20	0.57
1:A:171:GLN:HE22	1:A:319:ARG:NH1	2.03	0.57
1:D:468:ASP:OD2	1:D:677:LYS:HE3	2.05	0.57
1:D:602:ASN:HD21	1:D:617:VAL:H	1.52	0.57
1:A:396:VAL:O	1:A:705:LYS:HE2	2.05	0.56
1:A:625:ILE:HG12	1:A:683:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:ASP:HA	1:C:693:LEU:HD23	1.87	0.56
1:D:105:HIS:C	1:D:105:HIS:CD2	2.83	0.56
1:D:619:TYR:CZ	1:D:621:ASP:HB3	2.40	0.56
1:D:793:VAL:C	1:D:795:GLY:H	2.13	0.56
1:D:826:GLU:N	1:D:826:GLU:CD	2.62	0.56
3:J:113:DC:H2''	3:J:114:DA:C8	2.39	0.56
1:B:560:LYS:HE3	4:B:907:DTP:O3G	2.05	0.56
1:C:533:LEU:CD1	1:C:538:LEU:HG	2.29	0.56
1:C:752:MET:HG2	1:C:889:LEU:CD1	2.35	0.56
1:D:159:VAL:HG21	1:D:317:HIS:CE1	2.39	0.56
1:D:182:ILE:HD12	1:D:329:TYR:CD1	2.40	0.56
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.34	0.56
1:A:171:GLN:HE22	1:A:319:ARG:NH2	2.04	0.56
1:A:490:LEU:N	1:A:490:LEU:HD12	2.20	0.56
1:B:75:MET:O	1:B:78:ILE:HG22	2.05	0.56
1:B:491:ALA:HA	1:B:494:ARG:CZ	2.36	0.56
1:B:523:SER:O	1:B:527:LYS:HG3	2.04	0.56
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.87	0.56
1:C:403:ARG:HD3	5:C:937:HOH:O	2.06	0.56
1:D:188:TYR:CD2	1:D:190:PRO:HD3	2.40	0.56
1:D:396:VAL:HG23	1:D:396:VAL:O	2.05	0.56
1:D:619:TYR:CE1	1:D:621:ASP:HB3	2.40	0.56
1:D:710:LEU:HD12	1:D:726:LYS:HB3	1.85	0.56
1:D:734:LYS:HG3	1:D:735:SER:N	2.20	0.56
1:D:752:MET:CE	1:D:889:LEU:HD12	2.30	0.56
1:D:756:GLY:O	1:D:758:GLU:N	2.38	0.56
2:G:10:DA:H2''	2:G:11:DC:H5'	1.87	0.56
3:J:113:DC:H5'	3:J:113:DC:C6	2.40	0.56
1:A:115:ILE:HG22	1:A:136:ILE:HG12	1.86	0.56
1:C:412:LEU:HD13	1:C:415:LEU:CD1	2.33	0.56
1:D:623:ASP:C	1:D:623:ASP:OD2	2.48	0.56
3:H:114:DA:H2''	3:H:115:DA:O5'	2.05	0.56
1:A:785:ALA:CB	1:A:808:ILE:HD11	2.35	0.56
1:A:791:TYR:CD2	1:A:801:CYS:HA	2.41	0.56
1:B:720:TYR:CZ	1:B:724:LYS:HD2	2.40	0.56
1:C:546:GLN:C	1:C:548:THR:H	2.14	0.56
1:C:579:ASP:HB3	1:C:582:ASN:HD22	1.70	0.56
1:A:876:PHE:O	1:A:879:PRO:HD2	2.04	0.56
1:B:115:ILE:HG22	1:B:136:ILE:HG23	1.87	0.56
1:B:514:LEU:O	1:B:514:LEU:HD12	2.06	0.56
1:C:83:LEU:HD22	1:C:83:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PHE:HB3	1:A:683:MET:HE2	1.88	0.56
1:A:475:ILE:HD11	1:A:566:LEU:CD2	2.35	0.56
1:C:302:LYS:CD	1:C:326:ILE:HD12	2.36	0.56
1:D:277:TYR:O	1:D:281:SER:HB3	2.05	0.56
1:D:388:VAL:HG23	1:D:388:VAL:O	2.06	0.56
1:D:791:TYR:CE2	1:D:801:CYS:HA	2.40	0.56
1:D:808:ILE:HG22	1:D:812:ASN:HD21	1.71	0.56
1:A:412:LEU:HD22	1:A:415:LEU:HD13	1.86	0.56
1:A:428:GLU:CD	1:A:470:VAL:HG23	2.31	0.56
1:A:537:SER:OG	1:A:541:MET:HE3	2.05	0.56
1:C:286:PRO:HB3	1:C:782:VAL:HG21	1.88	0.56
1:C:808:ILE:CD1	1:C:830:VAL:HG11	2.36	0.56
1:A:66:ARG:HH11	1:A:66:ARG:HG3	1.70	0.56
1:B:101:ILE:HD13	1:B:352:LYS:HE2	1.88	0.56
1:B:395:PHE:HB2	1:B:591:GLN:HG3	1.88	0.56
1:C:81:GLU:HG2	1:C:83:LEU:CD2	2.35	0.56
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.20	0.56
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.40	0.56
1:C:145:ARG:HB2	1:C:147:TYR:HE1	1.69	0.56
1:C:216:TRP:HE1	1:C:274:ILE:HD12	1.70	0.56
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.88	0.56
1:A:739:LYS:HD3	1:A:742:GLN:OE1	2.06	0.56
1:B:511:ASP:CG	1:B:533:LEU:HD23	2.30	0.56
1:B:611:THR:HB	1:B:614:GLU:HG3	1.88	0.56
1:B:707:ARG:HD2	2:G:7:DA:H4'	1.88	0.56
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.88	0.56
1:C:891:TYR:CD2	1:C:892:GLU:HG3	2.41	0.56
1:D:15:ILE:HG23	1:D:65:MET:CE	2.32	0.56
1:D:444:ASN:HA	1:D:599:ARG:NE	2.21	0.56
1:C:305:TYR:OH	1:C:309:ILE:HG12	2.06	0.55
1:C:433:THR:N	1:C:462:MET:HE2	2.21	0.55
1:C:518:TYR:CD2	1:C:522:PHE:HZ	2.24	0.55
1:C:779:ILE:O	1:C:871:LEU:HD21	2.06	0.55
1:D:505:ASN:N	1:D:506:PRO:CD	2.67	0.55
3:J:110:DA:H2''	3:J:111:DT:H5'	1.87	0.55
1:C:623:ASP:OD2	3:J:115:DA:O3'	2.20	0.55
1:A:213:LEU:HD13	1:A:223:ILE:HD11	1.86	0.55
1:A:373:LEU:HD21	1:A:470:VAL:HG13	1.88	0.55
1:B:475:ILE:HD11	1:B:563:ILE:HG12	1.87	0.55
1:C:541:MET:O	1:C:545:ALA:N	2.39	0.55
1:D:85:MET:CA	1:D:380:ILE:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PRO:HB3	1:D:229:ARG:NH2	2.20	0.55
1:D:825:VAL:HG23	1:D:828:GLU:HB2	1.89	0.55
1:D:274:ILE:HG12	1:D:278:LYS:HE2	1.88	0.55
1:C:587:THR:HG22	1:C:588:THR:N	2.20	0.55
1:A:779:ILE:HG13	1:A:871:LEU:HD21	1.89	0.55
1:B:834:PRO:HD2	1:B:871:LEU:HD13	1.89	0.55
1:B:872:LEU:HD12	1:B:876:PHE:HB3	1.88	0.55
1:D:109:ARG:NH1	1:D:142:ILE:CD1	2.69	0.55
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.70	0.55
1:A:810:THR:CG2	1:A:841:PHE:HB3	2.36	0.55
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.88	0.55
1:B:753:LEU:HD12	1:B:753:LEU:N	2.21	0.55
1:C:604:TYR:O	1:C:608:VAL:HG23	2.06	0.55
1:C:634:ASP:C	1:C:636:VAL:H	2.12	0.55
1:D:198:LEU:C	1:D:200:GLU:N	2.61	0.55
1:D:408:MET:O	1:D:627:VAL:HG22	2.07	0.55
1:D:725:LEU:HD12	1:D:725:LEU:N	2.21	0.55
1:D:817:GLY:HA3	5:D:921:HOH:O	2.07	0.55
1:C:298:LEU:O	1:C:299:ASN:HB2	2.06	0.55
1:D:128:GLN:O	1:D:128:GLN:HG3	2.07	0.55
2:K:5:DG:H1'	2:K:6:DA:H5'	1.88	0.55
1:B:285:GLN:HG3	1:B:292:TYR:HE2	1.72	0.55
1:C:572:ASN:HD22	1:C:572:ASN:C	2.15	0.55
1:D:202:LEU:HD23	1:D:202:LEU:C	2.32	0.55
3:J:107:DG:H2''	3:J:108:DT:H5'	1.89	0.55
1:C:455:SER:HA	1:C:675:ASN:O	2.07	0.54
1:C:509:SER:O	1:C:511:ASP:N	2.38	0.54
1:D:61:LEU:HD23	1:D:61:LEU:O	2.06	0.54
1:D:402:ASN:ND2	1:D:403:ARG:O	2.40	0.54
2:I:13:DG:H2''	2:I:14:DC:H5'	1.89	0.54
1:A:48:LYS:HZ1	2:K:17:DC:P	2.30	0.54
1:A:730:LEU:HD13	1:A:883:PHE:CE1	2.42	0.54
1:B:353:ILE:HG13	1:B:354:GLN:O	2.06	0.54
1:B:779:ILE:HD12	1:B:871:LEU:HD23	1.88	0.54
1:C:498:ILE:HD12	1:C:501:GLU:OE2	2.07	0.54
1:D:105:HIS:CD2	1:D:106:THR:N	2.76	0.54
1:C:308:PRO:HG2	1:C:311:LYS:CG	2.37	0.54
1:C:322:SER:O	1:C:326:ILE:CG1	2.55	0.54
1:D:397:LYS:O	1:D:399:PRO:HD3	2.08	0.54
1:D:776:TYR:CG	1:D:863:LEU:HD11	2.42	0.54
3:L:103:DG:H2''	3:L:104:DG:O5'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:O	1:A:229:ARG:NH1	2.41	0.54
1:B:546:GLN:O	1:B:549:GLU:HB3	2.08	0.54
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.42	0.54
1:C:507:ASN:HB3	1:C:532:LYS:HG2	1.87	0.54
1:C:149:PHE:N	1:C:149:PHE:CD1	2.74	0.54
1:D:519:ARG:HB2	1:D:520:PHE:CD2	2.42	0.54
1:D:614:GLU:HB3	1:D:616:PHE:CE2	2.42	0.54
1:A:489:MET:HE1	1:A:553:MET:CG	2.37	0.54
1:A:513:PRO:HG2	1:A:540:GLU:CG	2.38	0.54
1:B:720:TYR:CE1	1:B:724:LYS:HD2	2.43	0.54
1:C:36:SER:HB3	1:C:59:ARG:HD3	1.89	0.54
1:C:806:ARG:NH1	1:C:844:LYS:HE2	2.22	0.54
1:D:92:TYR:CZ	1:D:96:THR:HG21	2.43	0.54
1:D:752:MET:HE3	1:D:760:LEU:HD22	1.89	0.54
2:I:9:DG:H2''	2:I:10:DA:C5'	2.38	0.54
2:I:11:DC:H2''	2:I:12:DA:H5'	1.89	0.54
1:A:249:ARG:HH21	1:A:251:LYS:NZ	2.05	0.54
1:A:279:LYS:C	1:A:280:PHE:CD1	2.82	0.54
1:A:280:PHE:CE2	1:A:343:LEU:HD22	2.42	0.54
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.89	0.54
1:C:491:ALA:C	1:C:493:GLN:H	2.16	0.54
1:C:78:ILE:CG1	1:C:80:LEU:HD23	2.38	0.54
1:C:272:ASP:OD1	1:C:274:ILE:HG22	2.08	0.54
1:C:489:MET:HA	5:C:940:HOH:O	2.06	0.54
3:H:105:DC:H2''	3:H:106:DT:O5'	2.08	0.54
3:J:102:DC:H1'	3:J:103:DG:H5'	1.89	0.54
1:B:274:ILE:HG23	1:B:275:ASP:N	2.22	0.54
1:B:835:LEU:HD23	1:B:866:MET:HA	1.90	0.54
1:C:548:THR:HG22	1:C:548:THR:O	2.07	0.54
1:D:180:SER:C	1:D:182:ILE:H	2.14	0.54
1:D:191:PHE:HE2	1:D:200:GLU:HG3	1.73	0.54
1:D:526:ILE:O	1:D:530:ILE:HG13	2.08	0.54
1:D:750:ARG:NH2	1:D:751:ARG:HG2	2.22	0.54
1:A:836:ARG:HH12	1:A:865:TRP:HA	1.73	0.54
1:B:597:ILE:HG21	1:B:667:PHE:CE2	2.43	0.54
1:C:41:CYS:HB2	1:C:42:PRO:HD2	1.90	0.54
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.90	0.54
1:C:458:PRO:HG2	1:C:592:MET:SD	2.48	0.54
1:D:136:ILE:CG2	1:D:149:PHE:HB2	2.31	0.54
1:D:260:ARG:HG2	1:D:260:ARG:HH11	1.73	0.54
1:D:830:VAL:HA	1:D:850:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:TYR:C	1:A:292:TYR:CD2	2.85	0.53
1:A:696:LYS:HB2	1:A:755:GLU:O	2.07	0.53
1:B:3:GLU:HG2	1:B:21:ASP:C	2.33	0.53
1:B:401:PRO:O	1:B:402:ASN:HB2	2.06	0.53
1:C:133:ILE:HD12	1:C:198:LEU:CD2	2.37	0.53
1:C:491:ALA:C	1:C:493:GLN:N	2.66	0.53
1:D:145:ARG:HB2	1:D:147:TYR:CE1	2.42	0.53
1:B:506:PRO:HB3	1:B:538:LEU:HD13	1.89	0.53
1:C:25:ARG:NE	1:C:27:ARG:HH12	2.07	0.53
1:C:302:LYS:HD3	1:C:326:ILE:HD12	1.90	0.53
1:C:518:TYR:HA	1:C:522:PHE:CE1	2.43	0.53
1:D:8:VAL:HG21	1:D:93:LEU:HD13	1.89	0.53
1:D:685:ARG:NH1	1:D:688:ILE:HG13	2.22	0.53
1:D:815:ILE:C	1:D:815:ILE:HD12	2.33	0.53
1:B:415:LEU:O	1:B:419:ILE:HG13	2.09	0.53
1:B:526:ILE:HG22	1:B:530:ILE:HD11	1.89	0.53
1:B:530:ILE:C	1:B:532:LYS:H	2.16	0.53
1:C:33:TYR:HD2	1:C:65:MET:CE	2.21	0.53
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.89	0.53
1:C:541:MET:HE1	1:C:542:LEU:HB2	1.88	0.53
1:D:528:GLU:OE2	1:D:531:LYS:HD2	2.08	0.53
1:D:826:GLU:O	1:D:828:GLU:HG3	2.08	0.53
2:I:15:DC:H2"	2:I:16:DG:N7	2.23	0.53
1:A:276:LEU:HD21	1:A:341:ILE:HD13	1.91	0.53
1:C:180:SER:HA	1:C:183:ILE:CD1	2.37	0.53
1:C:378:LYS:HE3	5:C:926:HOH:O	2.07	0.53
1:C:752:MET:HG2	1:C:889:LEU:HD12	1.90	0.53
1:C:870:VAL:HG12	1:C:874:LYS:HE2	1.91	0.53
1:D:109:ARG:CZ	1:D:142:ILE:HD11	2.38	0.53
1:D:145:ARG:HB2	1:D:147:TYR:HE1	1.73	0.53
1:D:685:ARG:NH2	1:D:717:GLY:H	2.05	0.53
2:I:3:DT:N3	4:J:2:DTP:N6	2.57	0.53
1:A:725:LEU:HD12	1:A:725:LEU:H	1.73	0.53
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.91	0.53
1:C:392:PRO:C	1:C:587:THR:HG21	2.33	0.53
1:D:227:TYR:HB3	1:D:263:ILE:HD13	1.90	0.53
1:D:417:PRO:O	1:D:421:ARG:HG3	2.08	0.53
1:D:444:ASN:HA	1:D:599:ARG:HE	1.72	0.53
1:A:517:ASP:OD2	1:A:519:ARG:HB3	2.09	0.53
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.90	0.53
1:C:38:PHE:CD1	1:C:38:PHE:N	2.75	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:HH21	1:D:319:ARG:HG2	1.74	0.53
1:D:830:VAL:CA	1:D:850:SER:HB2	2.39	0.53
2:G:16:DG:H2''	2:G:17:DC:C5'	2.39	0.53
1:A:301:GLY:O	1:A:330:ARG:NE	2.25	0.53
1:B:660:GLU:CB	1:B:661:PRO:HD3	2.37	0.53
1:C:271:LEU:HD21	1:C:356:GLN:HA	1.91	0.53
1:C:533:LEU:HD22	1:C:538:LEU:HA	1.90	0.53
1:D:309:ILE:HA	1:D:312:LEU:HB2	1.89	0.53
1:D:441:ASP:OD1	1:D:446:VAL:HB	2.08	0.53
1:D:734:LYS:HG2	1:D:736:SER:HB3	1.91	0.53
1:D:738:PRO:HG2	1:D:741:VAL:HG23	1.91	0.53
1:A:572:ASN:HD22	1:A:573:VAL:N	2.07	0.53
1:B:524:ASP:C	1:B:526:ILE:H	2.17	0.53
1:B:645:ASN:O	1:B:649:ASP:OD2	2.26	0.53
1:C:83:LEU:N	1:C:83:LEU:CD2	2.72	0.53
1:C:549:GLU:HA	5:C:940:HOH:O	2.08	0.53
1:B:416:TYR:HB2	1:B:417:PRO:HD3	1.91	0.53
1:D:523:SER:O	1:D:527:LYS:HG3	2.09	0.53
1:D:654:PHE:CD1	1:D:654:PHE:C	2.87	0.53
1:A:299:ASN:O	1:A:300:VAL:HB	2.09	0.53
1:B:433:THR:N	1:B:462:MET:HE2	2.23	0.53
1:C:138:HIS:C	1:C:138:HIS:CD2	2.87	0.53
1:C:279:LYS:HD2	1:C:280:PHE:CZ	2.43	0.53
1:C:355:ILE:O	1:C:358:VAL:HG13	2.09	0.53
1:C:541:MET:SD	1:C:542:LEU:N	2.82	0.53
1:D:894:LYS:HD2	1:D:894:LYS:N	2.24	0.53
3:L:105:DC:OP1	3:L:105:DC:H4'	2.08	0.53
1:A:713:TRP:CZ3	1:A:723:PRO:HB3	2.42	0.52
1:B:322:SER:O	1:B:326:ILE:HG12	2.09	0.52
1:B:395:PHE:HD2	1:B:594:LEU:HD23	1.74	0.52
1:B:873:GLU:HA	1:B:877:ILE:HG13	1.91	0.52
1:C:560:LYS:HG2	1:C:564:ASN:ND2	2.24	0.52
1:D:305:TYR:C	1:D:305:TYR:CD2	2.87	0.52
1:D:403:ARG:NH2	1:D:889:LEU:HD21	2.24	0.52
1:C:1:MET:HE1	1:C:4:PHE:HE1	1.75	0.52
1:C:148:VAL:C	1:C:149:PHE:CD1	2.87	0.52
1:C:578:TYR:OH	1:C:580:LEU:HD13	2.09	0.52
1:C:791:TYR:CE2	1:C:802:PRO:HD3	2.45	0.52
1:D:370:PHE:C	1:D:370:PHE:CD2	2.87	0.52
1:D:791:TYR:CD2	1:D:802:PRO:HD3	2.43	0.52
1:A:503:LEU:HG	1:A:538:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:GLY:HA2	1:A:753:LEU:HD22	1.92	0.52
1:A:731:GLU:HA	1:A:734:LYS:HD3	1.92	0.52
1:B:897:LEU:HD12	1:B:897:LEU:H	1.73	0.52
1:C:255:ASN:CG	1:C:256:MET:N	2.67	0.52
1:C:467:ARG:HH11	1:C:467:ARG:HG2	1.74	0.52
1:D:514:LEU:HD21	1:D:526:ILE:CG2	2.38	0.52
1:D:546:GLN:O	1:D:550:VAL:HG23	2.09	0.52
1:D:621:ASP:O	1:D:622:THR:HG22	2.09	0.52
1:A:105:HIS:CD2	1:A:106:THR:N	2.77	0.52
1:A:153:ASN:HD22	1:A:158:ASN:ND2	2.07	0.52
1:A:343:LEU:HD23	1:A:343:LEU:C	2.35	0.52
1:A:362:ILE:HD11	1:A:572:ASN:OD1	2.09	0.52
1:A:405:LYS:O	1:A:690:GLY:HA2	2.10	0.52
1:B:47:THR:OG1	1:B:48:LYS:N	2.40	0.52
1:C:109:ARG:HG3	1:C:109:ARG:HH11	1.74	0.52
1:C:482:ARG:O	1:C:483:LYS:C	2.52	0.52
1:D:260:ARG:HG2	1:D:260:ARG:NH1	2.24	0.52
1:A:365:TRP:CE2	1:A:566:LEU:HD12	2.45	0.52
1:A:599:ARG:HG2	1:A:599:ARG:HH11	1.75	0.52
1:B:149:PHE:HB3	1:B:197:LEU:HD21	1.92	0.52
1:C:48:LYS:HE3	1:C:49:TYR:CE2	2.44	0.52
1:C:506:PRO:HG3	1:C:538:LEU:CD1	2.39	0.52
1:C:533:LEU:HD22	1:C:538:LEU:HG	1.91	0.52
1:D:466:ASP:CG	1:D:467:ARG:H	2.16	0.52
1:D:517:ASP:C	1:D:519:ARG:H	2.17	0.52
1:D:779:ILE:HG22	1:D:871:LEU:HD21	1.90	0.52
1:D:785:ALA:O	1:D:827:GLY:N	2.42	0.52
1:A:153:ASN:ND2	1:A:158:ASN:ND2	2.57	0.52
1:A:249:ARG:HH21	1:A:251:LYS:HZ1	1.55	0.52
1:B:197:LEU:HD23	1:B:197:LEU:C	2.34	0.52
1:D:286:PRO:CG	1:D:733:GLN:HG3	2.38	0.52
1:D:741:VAL:HG11	1:D:875:THR:O	2.10	0.52
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.92	0.52
1:B:444:ASN:HA	1:B:599:ARG:HE	1.75	0.52
1:C:130:LYS:HE3	1:C:131:HIS:CE1	2.42	0.52
1:D:105:HIS:HA	1:D:108:ILE:HD12	1.92	0.52
1:D:140:ASP:HB3	1:D:143:ASP:HB2	1.91	0.52
1:D:362:ILE:HD13	1:D:575:PHE:HD1	1.74	0.52
1:D:416:TYR:O	1:D:420:ILE:HG13	2.10	0.52
1:D:685:ARG:HH22	1:D:717:GLY:H	1.57	0.52
1:A:397:LYS:O	1:A:399:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TYR:HA	1:A:491:ALA:HB3	1.92	0.52
1:A:785:ALA:HB1	1:A:808:ILE:HD11	1.92	0.52
1:B:85:MET:HA	1:B:380:ILE:HD11	1.91	0.52
1:B:253:ILE:HD13	1:B:254:GLU:N	2.23	0.52
1:D:362:ILE:CG2	1:D:363:LYS:N	2.73	0.52
1:A:548:THR:O	1:A:551:ALA:N	2.43	0.52
1:D:199:MET:HB3	1:D:234:PHE:CE2	2.45	0.52
1:D:202:LEU:HD23	1:D:202:LEU:O	2.09	0.52
1:D:458:PRO:CD	1:D:674:MET:HE2	2.40	0.52
1:A:284:ASN:HD22	1:A:285:GLN:N	2.07	0.52
1:B:536:LYS:HA	1:B:539:ASN:ND2	2.24	0.52
1:C:461:MET:HB3	1:C:463:TYR:CE1	2.44	0.52
1:D:273:TYR:HH	1:D:335:ASP:HA	1.74	0.52
1:D:286:PRO:HG3	1:D:733:GLN:HG3	1.90	0.52
1:A:339:GLN:OE1	1:A:339:GLN:HA	2.11	0.51
1:A:543:PHE:O	1:A:547:ARG:N	2.42	0.51
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.44	0.51
1:C:504:HIS:N	1:C:506:PRO:HD3	2.26	0.51
1:D:398:GLU:HB3	1:D:705:LYS:NZ	2.25	0.51
1:A:489:MET:HE1	1:A:553:MET:HG2	1.92	0.51
1:B:164:ILE:HD13	1:B:164:ILE:H	1.75	0.51
1:B:745:LEU:O	1:B:749:ILE:HG13	2.10	0.51
1:B:815:ILE:HD11	1:B:823:GLN:NE2	2.25	0.51
1:C:120:PRO:HD2	1:C:131:HIS:CD2	2.45	0.51
1:D:167:ALA:HB1	1:D:178:VAL:HG21	1.92	0.51
1:D:335:ASP:O	1:D:339:GLN:HA	2.10	0.51
1:D:413:THR:O	1:D:414:SER:C	2.53	0.51
1:D:459:ASN:ND2	1:D:585:ALA:HA	2.25	0.51
1:D:617:VAL:HG23	1:D:617:VAL:O	2.09	0.51
1:D:622:THR:HG23	1:D:623:ASP:N	2.24	0.51
1:D:739:LYS:HA	1:D:742:GLN:HB3	1.92	0.51
1:A:734:LYS:HE3	5:A:949:HOH:O	2.11	0.51
1:A:864:HIS:HD2	1:A:865:TRP:NE1	2.09	0.51
1:A:898:PHE:CD1	1:A:898:PHE:N	2.78	0.51
1:B:272:ASP:OD2	1:B:274:ILE:HG22	2.10	0.51
1:C:38:PHE:CZ	1:C:59:ARG:HG2	2.45	0.51
1:C:302:LYS:HZ3	1:C:302:LYS:CB	2.23	0.51
1:D:808:ILE:CG2	1:D:824:VAL:HG11	2.40	0.51
1:A:776:TYR:HB2	1:A:866:MET:HE1	1.93	0.51
1:B:101:ILE:CG2	1:B:349:TYR:HB3	2.40	0.51
1:C:468:ASP:HB3	1:C:677:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLN:HB3	1:D:356:GLN:OE1	2.10	0.51
1:D:398:GLU:CB	1:D:705:LYS:NZ	2.74	0.51
1:D:678:GLN:HG3	1:D:680:LEU:HG	1.92	0.51
1:A:542:LEU:C	1:A:542:LEU:HD12	2.36	0.51
1:B:3:GLU:HG2	1:B:21:ASP:HA	1.93	0.51
1:B:413:THR:O	1:B:414:SER:C	2.53	0.51
1:B:611:THR:CB	1:B:614:GLU:HG3	2.41	0.51
1:B:810:THR:CG2	1:B:841:PHE:HB3	2.40	0.51
1:D:274:ILE:HG23	1:D:275:ASP:N	2.26	0.51
1:D:536:LYS:HB2	1:D:536:LYS:NZ	2.25	0.51
1:C:248:THR:HB	1:C:264:THR:O	2.10	0.51
1:C:542:LEU:O	1:C:546:GLN:HG3	2.10	0.51
1:D:227:TYR:CB	1:D:263:ILE:HD13	2.40	0.51
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.22	0.51
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.93	0.51
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.24	0.51
1:B:163:SER:OG	1:B:166:ILE:HD13	2.09	0.51
1:B:181:GLU:CD	1:B:181:GLU:H	2.18	0.51
1:B:398:GLU:OE2	1:B:705:LYS:HE3	2.10	0.51
4:J:2:DTP:N3	4:J:2:DTP:H5'1	2.26	0.51
3:L:106:DT:H2''	3:L:107:DG:OP2	2.11	0.51
1:A:543:PHE:C	1:A:543:PHE:CD2	2.86	0.51
1:A:555:ALA:O	1:A:559:ARG:HG2	2.10	0.51
1:B:159:VAL:HG11	1:B:317:HIS:HB2	1.93	0.51
1:B:277:TYR:O	1:B:281:SER:HB2	2.10	0.51
1:B:518:TYR:HD2	1:B:545:ALA:HA	1.74	0.51
1:D:272:ASP:CG	1:D:274:ILE:HG22	2.36	0.51
1:A:162:TRP:CH2	1:A:164:ILE:HG13	2.45	0.51
1:A:566:LEU:HG	1:A:566:LEU:O	2.11	0.51
1:B:805:ILE:O	1:B:809:LEU:HD13	2.10	0.51
1:C:496:GLY:O	1:C:542:LEU:HD13	2.11	0.51
1:A:345:LEU:HD23	1:A:355:ILE:HG21	1.93	0.51
1:C:546:GLN:C	1:C:548:THR:N	2.68	0.51
1:C:634:ASP:C	1:C:636:VAL:N	2.68	0.51
1:D:124:PRO:HB2	1:D:225:TYR:HE1	1.76	0.51
1:D:416:TYR:HD1	1:D:586:ILE:CG2	2.24	0.51
1:D:555:ALA:O	1:D:559:ARG:HG2	2.11	0.51
2:E:16:DG:H2''	2:E:17:DC:C6	2.46	0.51
3:H:110:DA:H1'	3:H:111:DT:H5''	1.91	0.51
1:A:105:HIS:CD2	1:A:105:HIS:C	2.87	0.50
1:A:231:LYS:NZ	1:A:231:LYS:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:ILE:HG23	1:C:499:ILE:HD13	1.93	0.50
1:D:455:SER:OG	1:D:676:ASN:HA	2.11	0.50
1:D:559:ARG:HG2	1:D:559:ARG:HH11	1.76	0.50
1:A:41:CYS:CB	1:A:58:THR:HG23	2.42	0.50
1:A:365:TRP:CD2	1:A:566:LEU:HD12	2.46	0.50
1:A:423:VAL:O	1:A:424:ASN:HB3	2.12	0.50
1:B:180:SER:O	1:B:183:ILE:HG22	2.11	0.50
1:B:514:LEU:CD1	1:B:541:MET:HE1	2.41	0.50
1:B:529:LYS:HA	1:B:532:LYS:HD3	1.94	0.50
1:C:113:PHE:CD1	1:C:213:LEU:HD11	2.46	0.50
1:C:273:TYR:OH	1:C:335:ASP:HA	2.11	0.50
1:C:706:LYS:C	1:C:707:ARG:HG2	2.36	0.50
1:D:636:VAL:HG21	1:D:641:PHE:HZ	1.76	0.50
1:A:251:LYS:NZ	1:A:251:LYS:HB2	2.26	0.50
1:A:461:MET:HE2	1:A:461:MET:HA	1.93	0.50
1:A:559:ARG:HG2	1:A:559:ARG:HH11	1.76	0.50
1:B:143:ASP:OD2	1:B:208:LYS:NZ	2.38	0.50
1:B:202:LEU:O	1:B:206:GLN:HG2	2.11	0.50
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.45	0.50
1:C:302:LYS:HE3	1:C:326:ILE:HB	1.92	0.50
1:C:475:ILE:CG2	1:C:476:THR:N	2.74	0.50
1:D:504:HIS:C	1:D:506:PRO:HD3	2.35	0.50
1:B:154:SER:HB3	1:B:313:ARG:HH22	1.77	0.50
1:B:493:GLN:O	1:B:497:GLU:HG2	2.11	0.50
1:D:453:VAL:HG23	1:D:454:TYR:CD1	2.47	0.50
1:C:233:ILE:HG22	1:C:234:PHE:CD2	2.47	0.50
1:C:453:VAL:HG23	1:C:454:TYR:N	2.26	0.50
1:C:456:CYS:SG	1:C:462:MET:HG2	2.51	0.50
1:D:444:ASN:OD1	1:D:599:ARG:HD2	2.12	0.50
1:D:709:ALA:HB2	1:D:730:LEU:HD11	1.93	0.50
3:F:109:DC:H1'	3:F:110:DA:H5''	1.94	0.50
1:A:251:LYS:HB2	1:A:251:LYS:HZ2	1.77	0.50
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.24	0.50
1:C:878:LYS:HB3	1:C:879:PRO:HD3	1.94	0.50
1:D:4:PHE:HA	1:D:97:TYR:HE2	1.77	0.50
1:D:84:GLY:C	1:D:380:ILE:HD11	2.37	0.50
1:D:410:PHE:HB3	1:D:683:MET:HG2	1.94	0.50
1:D:775:ASN:OD1	1:D:777:ILE:HD11	2.12	0.50
3:J:114:DA:H2''	3:J:115:DA:O5'	2.10	0.50
1:B:469:GLY:O	1:B:472:PRO:HG2	2.12	0.50
1:B:499:ILE:HD12	1:B:545:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ILE:CD1	1:B:683:MET:SD	2.99	0.50
1:D:208:LYS:O	1:D:209:THR:C	2.54	0.50
1:D:224:PRO:HA	1:D:263:ILE:CD1	2.37	0.50
1:D:459:ASN:HD22	1:D:584:THR:HG22	1.75	0.50
1:D:636:VAL:HB	1:D:640:LYS:HD2	1.94	0.50
1:A:73:LYS:O	1:A:76:GLU:HB2	2.12	0.50
1:A:163:SER:HB3	1:A:318:GLN:OE1	2.12	0.50
1:A:206:GLN:OE1	1:A:241:ARG:HB3	2.12	0.50
1:C:109:ARG:HD2	1:C:209:THR:O	2.11	0.50
1:C:878:LYS:HB3	1:C:879:PRO:CD	2.42	0.50
1:D:256:MET:HB2	2:K:4:CTG:OP2	2.11	0.50
1:D:550:VAL:C	1:D:552:GLY:N	2.68	0.50
1:D:619:TYR:OH	1:D:621:ASP:HB3	2.11	0.50
1:D:648:VAL:CG1	1:D:719:ARG:NH2	2.75	0.50
1:A:113:PHE:CE1	1:A:218:VAL:CG2	2.95	0.50
1:C:62:PHE:CD1	1:C:62:PHE:N	2.79	0.50
1:C:542:LEU:C	1:C:546:GLN:NE2	2.68	0.50
1:D:150:ASP:OD1	1:D:151:LEU:N	2.45	0.50
1:D:428:GLU:OE2	1:D:428:GLU:N	2.45	0.50
1:D:777:ILE:HG22	1:D:848:TRP:HH2	1.77	0.50
1:A:193:ASN:HD21	1:A:196:GLU:CD	2.20	0.49
1:A:388:VAL:HG22	1:A:573:VAL:HG21	1.94	0.49
1:B:444:ASN:HA	1:B:599:ARG:NE	2.27	0.49
1:B:686:GLU:HG3	1:B:715:MET:SD	2.52	0.49
1:C:493:GLN:HG2	1:C:549:GLU:OE1	2.12	0.49
1:D:15:ILE:CG1	1:D:31:VAL:HG22	2.42	0.49
1:D:221:PHE:O	1:D:224:PRO:HD2	2.12	0.49
1:D:292:TYR:CD1	1:D:292:TYR:C	2.90	0.49
1:A:731:GLU:O	1:A:734:LYS:HG2	2.12	0.49
1:A:785:ALA:C	1:A:786:ASN:HD22	2.20	0.49
1:B:518:TYR:CD2	1:B:545:ALA:HA	2.47	0.49
1:C:499:ILE:HB	1:C:541:MET:CE	2.42	0.49
1:D:138:HIS:C	1:D:138:HIS:CD2	2.90	0.49
1:D:243:SER:C	1:D:245:HIS:H	2.20	0.49
1:D:455:SER:HA	1:D:675:ASN:O	2.11	0.49
1:B:369:ILE:HG22	1:B:373:LEU:CD1	2.41	0.49
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.43	0.49
1:C:444:ASN:HA	1:C:599:ARG:NE	2.26	0.49
1:C:711:ASN:ND2	1:C:754:GLN:NE2	2.50	0.49
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.12	0.49
1:C:338:ARG:O	1:C:339:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LYS:HB3	1:C:620:GLY:H	1.77	0.49
1:D:16:PHE:HB3	1:D:245:HIS:NE2	2.27	0.49
1:D:105:HIS:HD2	1:D:106:THR:N	2.09	0.49
1:D:170:LEU:HG	1:D:171:GLN:N	2.28	0.49
1:A:711:ASN:HD21	1:A:723:PRO:HB2	1.77	0.49
1:B:471:VAL:N	1:B:472:PRO:HD2	2.28	0.49
1:C:44:SER:O	1:C:46:ALA:N	2.45	0.49
1:C:249:ARG:HH11	1:C:249:ARG:HG3	1.78	0.49
1:C:685:ARG:HD2	1:C:685:ARG:C	2.36	0.49
1:D:416:TYR:HE1	1:D:587:THR:HA	1.77	0.49
1:D:491:ALA:HB1	1:D:520:PHE:HA	1.94	0.49
1:B:164:ILE:H	1:B:164:ILE:CD1	2.26	0.49
1:B:313:ARG:O	1:B:317:HIS:HB2	2.13	0.49
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.42	0.49
1:C:163:SER:H	1:C:318:GLN:HE22	1.60	0.49
1:C:533:LEU:HB3	1:C:538:LEU:CG	2.43	0.49
1:C:614:GLU:HB3	1:C:616:PHE:CE1	2.48	0.49
1:C:749:ILE:O	1:C:753:LEU:HG	2.12	0.49
1:D:142:ILE:HG13	1:D:143:ASP:N	2.27	0.49
1:D:197:LEU:HD13	1:D:197:LEU:C	2.37	0.49
1:D:204:PHE:O	1:D:207:GLN:HB3	2.12	0.49
2:G:12:DA:H2''	2:G:13:DG:H8	1.76	0.49
1:A:559:ARG:O	1:A:563:ILE:HG13	2.11	0.49
1:B:5:TYR:HB3	1:B:97:TYR:CE2	2.48	0.49
1:C:116:GLU:CB	1:C:135:ALA:HB3	2.37	0.49
1:C:147:TYR:HB3	1:C:149:PHE:HE1	1.78	0.49
1:C:388:VAL:O	1:C:388:VAL:HG23	2.13	0.49
1:C:467:ARG:HG2	1:C:467:ARG:NH1	2.27	0.49
1:C:533:LEU:HD13	1:C:538:LEU:CG	2.34	0.49
1:D:886:ALA:C	1:D:888:LYS:H	2.20	0.49
1:A:399:PRO:O	1:A:401:PRO:HD3	2.12	0.49
1:A:505:ASN:HD22	1:A:505:ASN:C	2.20	0.49
1:B:19:TYR:CZ	1:B:27:ARG:HB2	2.47	0.49
1:C:508:LEU:O	1:C:509:SER:HB3	2.12	0.49
1:C:533:LEU:HB3	1:C:538:LEU:HG	1.94	0.49
1:C:686:GLU:HA	1:C:686:GLU:OE2	2.13	0.49
1:D:438:PRO:HG2	1:D:441:ASP:HB2	1.94	0.49
1:D:447:ALA:O	1:D:673:TYR:OH	2.28	0.49
2:I:5:DG:H2''	2:I:6:DA:O5'	2.12	0.49
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.77	0.49
1:C:42:PRO:HG2	1:C:45:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD1	1:C:142:ILE:HB	2.12	0.49
1:C:542:LEU:HA	1:C:545:ALA:HB3	1.93	0.49
1:D:297:GLU:HG3	1:D:337:LYS:HD3	1.95	0.49
1:D:398:GLU:HA	1:D:705:LYS:NZ	2.25	0.49
1:D:748:CYS:O	1:D:752:MET:HG3	2.13	0.49
2:K:11:DC:H2''	2:K:12:DA:C8	2.48	0.49
1:A:495:ASN:C	1:A:497:GLU:N	2.69	0.48
1:A:700:GLY:HA3	1:A:710:LEU:HD23	1.95	0.48
1:B:133:ILE:HD12	1:B:198:LEU:HD21	1.95	0.48
1:B:422:GLN:HG3	1:B:678:GLN:O	2.13	0.48
1:B:604:TYR:CZ	1:B:608:VAL:HG21	2.47	0.48
1:C:324:ASN:C	1:C:324:ASN:ND2	2.70	0.48
1:D:290:LEU:O	1:D:294:SER:HB2	2.13	0.48
1:D:347:MET:HB2	1:D:558:ASN:OD1	2.11	0.48
2:I:13:DG:H2''	2:I:14:DC:C5'	2.44	0.48
1:A:456:CYS:SG	1:A:462:MET:HG2	2.53	0.48
1:C:219:GLU:HG2	1:C:219:GLU:O	2.11	0.48
1:C:244:PRO:HG2	1:C:267:GLY:HA3	1.95	0.48
1:C:402:ASN:HD22	1:C:403:ARG:H	1.57	0.48
1:D:702:TRP:CD1	1:D:708:TYR:HB3	2.48	0.48
1:A:402:ASN:HA	1:A:886:ALA:O	2.13	0.48
1:A:408:MET:HE1	1:A:659:MET:CE	2.34	0.48
1:A:732:THR:OG1	1:A:733:GLN:NE2	2.26	0.48
1:A:733:GLN:O	3:F:112:DT:H5''	2.14	0.48
1:B:747:GLU:OE1	1:B:747:GLU:HA	2.13	0.48
1:B:897:LEU:HD12	1:B:897:LEU:N	2.27	0.48
1:C:265:LEU:HD12	1:C:268:ILE:HD12	1.95	0.48
1:D:257:TYR:CD2	3:L:112:DT:H72	2.48	0.48
1:D:777:ILE:HG22	1:D:848:TRP:CH2	2.48	0.48
1:A:401:PRO:O	1:A:402:ASN:HB2	2.13	0.48
1:C:301:GLY:O	1:C:330:ARG:HD2	2.13	0.48
1:C:489:MET:C	1:C:491:ALA:N	2.72	0.48
1:D:109:ARG:HH21	1:D:208:LYS:HG2	1.78	0.48
1:D:648:VAL:CG1	1:D:719:ARG:HH21	2.24	0.48
1:D:739:LYS:NZ	1:D:743:LYS:HD2	2.28	0.48
1:B:707:ARG:HD2	2:G:7:DA:O3'	2.13	0.48
1:B:796:PHE:HB3	1:B:797:PRO:HD2	1.95	0.48
1:D:166:ILE:HG22	1:D:166:ILE:O	2.12	0.48
1:D:305:TYR:C	1:D:305:TYR:HD2	2.21	0.48
1:D:313:ARG:HG2	1:D:313:ARG:HH21	1.77	0.48
1:D:654:PHE:CE1	1:D:659:MET:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:GLN:NE2	1:D:893:LYS:HA	2.28	0.48
1:A:760:LEU:HD23	1:A:891:TYR:HA	1.94	0.48
1:B:177:GLU:HB3	1:B:303:LEU:HD11	1.95	0.48
1:B:553:MET:O	1:B:557:ILE:HG12	2.13	0.48
1:C:401:PRO:O	1:C:402:ASN:HB2	2.12	0.48
1:D:52:ILE:O	1:D:428:GLU:HG3	2.14	0.48
1:D:533:LEU:HB2	1:D:538:LEU:HD21	1.96	0.48
1:B:256:MET:HG2	1:B:257:TYR:CE2	2.48	0.48
1:B:481:GLN:OE1	1:B:559:ARG:NH1	2.47	0.48
1:B:540:GLU:O	1:B:544:ARG:HG3	2.13	0.48
1:C:121:ASP:C	1:C:819:ILE:HG12	2.39	0.48
1:C:404:TYR:CD1	1:C:618:LEU:HD22	2.48	0.48
1:C:443:ILE:O	1:C:599:ARG:NH2	2.45	0.48
1:C:499:ILE:O	1:C:503:LEU:HG	2.12	0.48
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.35	0.48
1:D:85:MET:N	1:D:380:ILE:HD11	2.29	0.48
1:D:180:SER:O	1:D:182:ILE:N	2.44	0.48
1:D:516:VAL:HG22	1:D:517:ASP:N	2.28	0.48
2:G:15:DC:H2''	2:G:16:DG:OP2	2.12	0.48
2:K:9:DG:H2''	2:K:10:DA:OP2	2.13	0.48
1:A:3:GLU:HG2	1:A:21:ASP:HA	1.96	0.48
1:B:179:PRO:HB2	1:B:181:GLU:OE1	2.13	0.48
1:C:506:PRO:HG3	1:C:538:LEU:HD11	1.96	0.48
1:D:309:ILE:HG22	1:D:312:LEU:HD22	1.95	0.48
1:D:803:PHE:C	1:D:803:PHE:CD2	2.91	0.48
1:A:326:ILE:O	1:A:330:ARG:HG2	2.14	0.48
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.44	0.48
1:C:42:PRO:CG	1:C:45:GLN:HG3	2.44	0.48
1:C:540:GLU:OE1	1:C:540:GLU:HA	2.13	0.48
1:D:423:VAL:O	1:D:424:ASN:HB3	2.14	0.48
1:D:758:GLU:HG3	1:D:759:SER:H	1.78	0.48
1:A:518:TYR:O	1:A:519:ARG:C	2.57	0.48
1:A:870:VAL:O	1:A:874:LYS:CG	2.62	0.48
1:B:538:LEU:O	1:B:542:LEU:HB2	2.14	0.48
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.25	0.48
1:D:826:GLU:CD	1:D:826:GLU:H	2.21	0.48
1:D:878:LYS:O	1:D:881:GLU:HG3	2.14	0.48
2:I:9:DG:H1'	2:I:10:DA:H5''	1.94	0.48
1:A:104:ASP:OD2	1:A:106:THR:HB	2.14	0.47
1:A:671:CYS:SG	1:A:676:ASN:HB2	2.54	0.47
1:A:829:LYS:N	1:A:829:LYS:HE3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:MET:HG3	3:H:114:DA:H3'	1.95	0.47
1:C:68:ALA:O	1:C:72:ILE:HG13	2.14	0.47
1:C:757:GLU:O	1:C:761:GLN:HG3	2.13	0.47
1:D:644:THR:O	1:D:648:VAL:HG23	2.14	0.47
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.95	0.47
1:B:41:CYS:HB2	1:B:42:PRO:HD2	1.96	0.47
1:B:126:PRO:HB2	1:B:224:PRO:HB2	1.96	0.47
1:C:38:PHE:CE2	1:C:59:ARG:HG2	2.49	0.47
1:D:702:TRP:NE1	1:D:708:TYR:HB3	2.28	0.47
2:I:16:DG:H2''	2:I:17:DC:O5'	2.14	0.47
1:A:102:LYS:HD3	1:A:102:LYS:C	2.39	0.47
1:B:270:VAL:O	1:B:271:LEU:HD12	2.12	0.47
1:B:815:ILE:HD11	1:B:823:GLN:HE22	1.79	0.47
1:C:252:VAL:HA	1:C:261:GLU:HA	1.96	0.47
1:D:2:LYS:NZ	1:D:2:LYS:HB3	2.29	0.47
1:D:153:ASN:O	1:D:154:SER:HB2	2.14	0.47
1:D:194:GLU:OE1	1:D:198:LEU:HD21	2.13	0.47
1:D:414:SER:O	1:D:417:PRO:HD2	2.13	0.47
2:E:11:DC:H1'	2:E:12:DA:H5''	1.96	0.47
3:L:111:DT:H2''	3:L:112:DT:C5'	2.43	0.47
1:C:351:ALA:O	1:C:352:LYS:HB2	2.14	0.47
1:C:494:ARG:HG2	1:C:494:ARG:HH11	1.79	0.47
1:C:527:LYS:C	1:C:529:LYS:H	2.22	0.47
1:C:668:ARG:HH11	1:C:668:ARG:HG2	1.80	0.47
1:D:104:ASP:O	1:D:104:ASP:CG	2.57	0.47
1:D:164:ILE:HD13	1:D:164:ILE:N	2.07	0.47
1:D:411:ASP:OD2	1:D:624:SER:HB3	2.14	0.47
1:A:194:GLU:OE1	1:A:229:ARG:NE	2.43	0.47
1:A:231:LYS:HB3	1:A:231:LYS:HZ3	1.79	0.47
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.43	0.47
1:B:283:THR:HG23	1:B:283:THR:O	2.15	0.47
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.96	0.47
1:B:797:PRO:HG3	1:B:806:ARG:NH1	2.30	0.47
1:C:59:ARG:HG3	1:C:59:ARG:NH1	2.28	0.47
1:C:373:LEU:HD12	1:C:380:ILE:HG22	1.96	0.47
1:C:450:PRO:HB2	1:C:456:CYS:SG	2.55	0.47
1:D:51:ASP:OD1	1:D:53:TYR:HB2	2.15	0.47
1:D:238:THR:O	1:D:238:THR:HG22	2.14	0.47
1:D:723:PRO:C	1:D:724:LYS:HD2	2.40	0.47
1:A:433:THR:HG22	1:A:461:MET:HE1	1.97	0.47
1:A:510:VAL:O	1:A:510:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:GLU:HG3	1:B:617:VAL:HG11	1.97	0.47
1:C:34:LYS:HD3	1:C:61:LEU:HD21	1.95	0.47
1:C:900:MET:HE2	1:C:901:PHE:CE2	2.50	0.47
1:D:300:VAL:HG23	1:D:330:ARG:HE	1.79	0.47
1:D:714:ASP:OD2	1:D:719:ARG:HG2	2.15	0.47
2:K:2:DG:N2	5:K:130:HOH:O	2.46	0.47
1:A:403:ARG:C	1:A:404:TYR:CD2	2.93	0.47
1:A:518:TYR:CE2	1:A:545:ALA:HB2	2.50	0.47
1:A:572:ASN:HD22	1:A:572:ASN:C	2.23	0.47
1:A:731:GLU:HG3	1:A:879:PRO:CB	2.40	0.47
1:C:154:SER:C	1:C:156:TYR:H	2.23	0.47
1:C:302:LYS:HG2	1:C:323:TYR:CE2	2.50	0.47
1:D:135:ALA:C	1:D:136:ILE:HG22	2.38	0.47
1:D:179:PRO:HB2	1:D:182:ILE:CG2	2.44	0.47
3:J:114:DA:H2''	3:J:115:DA:C5'	2.45	0.47
2:K:5:DG:H2''	2:K:6:DA:O5'	2.14	0.47
1:A:249:ARG:HE	1:A:249:ARG:HB2	1.54	0.47
1:A:513:PRO:HG2	1:A:540:GLU:HG2	1.97	0.47
1:C:455:SER:OG	1:C:676:ASN:HA	2.14	0.47
1:C:495:ASN:HB3	1:C:522:PHE:CD1	2.50	0.47
1:C:518:TYR:C	1:C:520:PHE:H	2.21	0.47
1:D:412:LEU:HD12	1:D:415:LEU:HD22	1.97	0.47
1:D:808:ILE:O	1:D:812:ASN:ND2	2.48	0.47
1:A:408:MET:CE	1:A:659:MET:HE1	2.34	0.47
1:B:659:MET:O	1:B:660:GLU:C	2.57	0.47
1:C:153:ASN:HB3	1:C:158:ASN:OD1	2.15	0.47
1:C:556:GLN:NE2	1:C:556:GLN:C	2.73	0.47
1:C:822:PRO:HD2	1:C:855:THR:OG1	2.14	0.47
1:D:347:MET:HE2	1:D:558:ASN:ND2	2.30	0.47
1:D:629:ALA:O	1:D:630:ASP:C	2.57	0.47
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.40	0.47
1:B:197:LEU:C	1:B:197:LEU:CD2	2.88	0.47
1:B:488:TYR:CD2	1:B:519:ARG:HD2	2.50	0.47
1:C:13:ASP:HA	1:C:65:MET:HG3	1.97	0.47
1:C:139:TYR:C	1:C:139:TYR:CD1	2.93	0.47
1:C:163:SER:HB3	1:C:166:ILE:CD1	2.45	0.47
1:C:312:LEU:HD12	1:C:312:LEU:O	2.14	0.47
1:C:497:GLU:HG2	1:C:497:GLU:O	2.15	0.47
1:C:503:LEU:CD2	1:C:538:LEU:HD22	2.45	0.47
1:A:4:PHE:CZ	1:A:20:ILE:HG13	2.51	0.46
1:A:15:ILE:HG12	1:A:65:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HB3	1:A:48:LYS:HZ3	1.79	0.46
1:D:553:MET:O	1:D:556:GLN:HG3	2.15	0.46
1:A:297:GLU:OE2	1:A:337:LYS:NZ	2.43	0.46
1:B:3:GLU:HG2	1:B:22:SER:N	2.31	0.46
1:C:460:GLY:C	1:C:461:MET:HE2	2.40	0.46
1:C:877:ILE:O	1:C:878:LYS:C	2.58	0.46
1:D:19:TYR:CZ	1:D:27:ARG:HB2	2.50	0.46
1:D:154:SER:C	1:D:156:TYR:N	2.74	0.46
1:D:470:VAL:HG13	1:D:471:VAL:N	2.30	0.46
1:D:579:ASP:C	1:D:579:ASP:OD2	2.58	0.46
2:K:5:DG:C6	2:K:6:DA:C2	3.03	0.46
1:A:335:ASP:OD2	1:A:341:ILE:HG12	2.15	0.46
1:A:402:ASN:HB3	1:A:404:TYR:CE2	2.51	0.46
1:A:642:ARG:CZ	1:A:646:HIS:CD2	2.99	0.46
1:B:44:SER:O	1:B:46:ALA:N	2.48	0.46
1:C:384:ARG:HB2	1:C:386:HIS:CE1	2.50	0.46
1:C:490:LEU:O	1:C:494:ARG:CG	2.63	0.46
1:C:507:ASN:CB	1:C:532:LYS:HA	2.44	0.46
1:C:659:MET:O	1:C:663:ILE:HG13	2.16	0.46
1:D:123:PHE:CD1	1:D:124:PRO:HD2	2.49	0.46
1:D:293:ILE:HD12	1:D:293:ILE:C	2.40	0.46
1:D:493:GLN:C	1:D:495:ASN:H	2.23	0.46
1:A:693:LEU:HA	5:A:929:HOH:O	2.15	0.46
1:A:898:PHE:H	1:A:898:PHE:HD1	1.63	0.46
1:B:415:LEU:HD11	1:B:419:ILE:HD11	1.97	0.46
1:B:423:VAL:O	1:B:424:ASN:HB3	2.15	0.46
1:B:625:ILE:O	1:B:625:ILE:HG13	2.15	0.46
1:B:785:ALA:CB	1:B:808:ILE:HD11	2.45	0.46
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.30	0.46
1:D:151:LEU:HD21	1:D:193:ASN:O	2.15	0.46
1:D:194:GLU:O	1:D:195:LYS:C	2.58	0.46
1:D:289:SER:O	1:D:293:ILE:HG13	2.15	0.46
1:D:500:LYS:C	1:D:502:ALA:H	2.22	0.46
1:D:522:PHE:O	1:D:527:LYS:HE3	2.15	0.46
1:A:274:ILE:O	1:A:278:LYS:HG3	2.15	0.46
1:A:805:ILE:HA	1:A:808:ILE:HD12	1.98	0.46
1:A:854:ILE:CG2	1:A:859:LYS:HG3	2.45	0.46
1:B:503:LEU:HD12	1:B:542:LEU:CD2	2.45	0.46
1:B:531:LYS:NZ	1:B:531:LYS:HB3	2.31	0.46
1:B:726:LYS:NZ	1:B:728:MET:HE2	2.31	0.46
1:C:130:LYS:HG3	1:C:131:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:SER:O	1:C:417:PRO:HD2	2.15	0.46
1:C:872:LEU:HD11	1:C:876:PHE:CD2	2.50	0.46
1:D:709:ALA:HA	1:D:726:LYS:O	2.16	0.46
1:A:147:TYR:CE2	1:A:187:ILE:HD12	2.50	0.46
1:B:129:ALA:HA	1:B:225:TYR:CZ	2.51	0.46
1:B:163:SER:N	1:B:318:GLN:HE22	2.10	0.46
1:B:299:ASN:O	1:B:300:VAL:HB	2.16	0.46
1:B:523:SER:HA	1:B:527:LYS:HE3	1.98	0.46
1:C:300:VAL:HG22	1:C:330:ARG:NH1	2.23	0.46
1:C:361:PRO:HD2	2:I:2:DG:P	2.55	0.46
1:C:413:THR:O	1:C:414:SER:C	2.59	0.46
1:C:523:SER:HB2	1:C:526:ILE:HG13	1.97	0.46
1:D:398:GLU:CB	1:D:705:LYS:HE3	2.39	0.46
1:A:81:GLU:OE2	1:A:83:LEU:CG	2.64	0.46
1:A:138:HIS:HE1	5:A:919:HOH:O	1.98	0.46
1:B:116:GLU:HG2	1:B:320:TYR:CZ	2.51	0.46
1:B:221:PHE:O	1:B:224:PRO:HD2	2.16	0.46
1:B:458:PRO:HB2	1:B:588:THR:HG22	1.97	0.46
1:C:453:VAL:CG2	1:C:454:TYR:N	2.79	0.46
1:D:7:THR:OG1	1:D:18:ARG:HD3	2.15	0.46
1:D:188:TYR:CE2	1:D:190:PRO:HD3	2.51	0.46
1:A:64:ASN:ND2	1:A:67:ASP:CG	2.74	0.46
1:A:85:MET:HA	1:A:380:ILE:HD11	1.98	0.46
1:A:642:ARG:HB2	1:A:642:ARG:CZ	2.45	0.46
1:A:801:CYS:SG	1:A:805:ILE:HG22	2.56	0.46
1:D:297:GLU:OE1	1:D:297:GLU:HA	2.15	0.46
1:D:347:MET:HE2	1:D:558:ASN:HD21	1.80	0.46
1:D:459:ASN:ND2	1:D:585:ALA:CA	2.78	0.46
2:G:16:DG:C2'	2:G:17:DC:H5''	2.46	0.46
1:C:147:TYR:HB3	1:C:149:PHE:CE1	2.51	0.46
1:C:433:THR:O	1:C:462:MET:SD	2.74	0.46
1:C:461:MET:HB3	1:C:463:TYR:HE1	1.80	0.46
1:D:4:PHE:HA	1:D:97:TYR:CE2	2.51	0.46
1:D:426:SER:OG	1:D:427:PRO:HD2	2.16	0.46
1:D:498:ILE:O	1:D:498:ILE:HG22	2.16	0.46
1:D:572:ASN:O	1:D:578:TYR:HB2	2.16	0.46
1:B:487:GLY:O	1:B:491:ALA:HB2	2.15	0.46
1:C:49:TYR:HE1	1:C:59:ARG:HB2	1.81	0.46
1:C:475:ILE:HD13	1:C:566:LEU:HD22	1.98	0.46
1:D:85:MET:HE2	1:D:380:ILE:HD13	1.97	0.46
1:D:550:VAL:C	1:D:552:GLY:H	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:848:TRP:CD1	1:D:848:TRP:H	2.34	0.46
3:L:111:DT:C2'	3:L:112:DT:H5''	2.45	0.46
1:A:376:GLN:NE2	1:A:378:LYS:HD2	2.31	0.45
1:A:490:LEU:HD23	1:A:494:ARG:HD3	1.98	0.45
1:A:713:TRP:CE3	1:A:723:PRO:HB3	2.51	0.45
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.51	0.45
1:B:145:ARG:HD3	1:B:185:LYS:O	2.17	0.45
1:B:489:MET:HE2	1:B:553:MET:HB2	1.98	0.45
1:B:597:ILE:HG21	1:B:667:PHE:CZ	2.51	0.45
1:B:876:PHE:O	1:B:879:PRO:HG2	2.15	0.45
1:C:159:VAL:CG1	1:C:160:GLU:N	2.76	0.45
1:C:542:LEU:C	1:C:544:ARG:H	2.24	0.45
1:C:659:MET:O	1:C:660:GLU:C	2.59	0.45
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.51	0.45
1:D:221:PHE:HE2	1:D:225:TYR:HD1	1.64	0.45
1:D:254:GLU:HB3	1:D:259:SER:HB3	1.98	0.45
1:D:491:ALA:O	1:D:495:ASN:CB	2.52	0.45
1:A:303:LEU:HB3	5:A:907:HOH:O	2.15	0.45
1:A:599:ARG:HG2	1:A:599:ARG:NH1	2.32	0.45
1:B:524:ASP:C	1:B:526:ILE:N	2.75	0.45
1:B:622:THR:HB	3:H:115:DA:O3'	2.15	0.45
1:C:250:VAL:HG22	1:C:263:ILE:CD1	2.47	0.45
1:D:19:TYR:CE1	1:D:27:ARG:HB2	2.51	0.45
1:D:191:PHE:CD1	1:D:197:LEU:HD23	2.51	0.45
1:D:776:TYR:CD2	1:D:863:LEU:HD11	2.50	0.45
1:D:883:PHE:N	1:D:883:PHE:HD2	2.13	0.45
1:A:412:LEU:HG	1:A:683:MET:CG	2.45	0.45
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.98	0.45
1:B:324:ASN:C	1:B:324:ASN:HD22	2.23	0.45
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.98	0.45
1:B:750:ARG:HG2	1:B:754:GLN:NE2	2.31	0.45
1:C:221:PHE:C	1:C:224:PRO:HD2	2.41	0.45
1:D:348:GLY:HA3	1:D:355:ILE:HD13	1.99	0.45
1:D:599:ARG:HH11	1:D:599:ARG:CG	2.30	0.45
1:D:631:LYS:HE2	1:D:631:LYS:HA	1.97	0.45
1:D:747:GLU:CD	1:D:750:ARG:HE	2.24	0.45
3:L:103:DG:H8	3:L:103:DG:OP2	2.00	0.45
1:A:455:SER:OG	1:A:676:ASN:HA	2.17	0.45
1:B:89:LYS:HB2	1:B:89:LYS:HE3	1.62	0.45
1:C:395:PHE:CE2	1:C:595:GLN:HG3	2.52	0.45
1:C:397:LYS:HE2	1:C:598:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.98	0.45
1:C:854:ILE:HG22	1:C:859:LYS:CD	2.47	0.45
1:C:894:LYS:HD3	1:C:894:LYS:HA	1.68	0.45
1:D:198:LEU:N	1:D:198:LEU:CD2	2.79	0.45
1:D:771:PHE:CE2	1:D:872:LEU:HB2	2.52	0.45
1:D:811:TYR:O	1:D:814:ALA:HB3	2.15	0.45
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.99	0.45
1:A:592:MET:HE1	1:A:674:MET:CG	2.46	0.45
1:A:644:THR:O	1:A:648:VAL:HG23	2.17	0.45
1:A:836:ARG:HG3	1:A:836:ARG:NH1	2.31	0.45
1:B:517:ASP:C	1:B:519:ARG:H	2.25	0.45
1:B:535:ALA:O	1:B:539:ASN:ND2	2.49	0.45
1:B:800:LYS:O	1:B:800:LYS:HG2	2.16	0.45
1:C:279:LYS:HD2	1:C:280:PHE:CE2	2.52	0.45
1:D:153:ASN:ND2	1:D:192:ASP:O	2.50	0.45
1:D:227:TYR:HB3	1:D:263:ILE:CD1	2.47	0.45
1:D:227:TYR:CD2	1:D:263:ILE:HD13	2.51	0.45
1:D:283:THR:HG23	1:D:283:THR:O	2.16	0.45
1:D:649:ASP:CG	1:D:719:ARG:HH12	2.23	0.45
1:A:112:ASN:ND2	1:A:214:THR:HG23	2.31	0.45
1:A:337:LYS:HE3	1:A:338:ARG:HD3	1.97	0.45
1:A:634:ASP:C	1:A:636:VAL:H	2.23	0.45
1:C:149:PHE:N	1:C:149:PHE:HD1	2.13	0.45
1:D:109:ARG:HH21	1:D:208:LYS:CG	2.30	0.45
1:D:194:GLU:OE2	1:D:229:ARG:NH2	2.48	0.45
1:D:752:MET:HE3	1:D:760:LEU:CD2	2.47	0.45
2:I:12:DA:H1'	2:I:13:DG:C8	2.52	0.45
1:A:38:PHE:N	1:A:38:PHE:CD1	2.85	0.45
1:A:48:LYS:HB3	1:A:48:LYS:NZ	2.32	0.45
1:B:303:LEU:HB3	1:B:319:ARG:NH2	2.30	0.45
1:B:785:ALA:HB2	1:B:808:ILE:HD11	1.98	0.45
1:C:589:PHE:C	1:C:589:PHE:CD1	2.94	0.45
1:D:326:ILE:O	1:D:330:ARG:HG2	2.16	0.45
1:D:503:LEU:HD23	1:D:503:LEU:C	2.41	0.45
1:D:619:TYR:CD1	1:D:619:TYR:C	2.94	0.45
1:A:237:SER:HB2	5:A:918:HOH:O	2.17	0.45
1:A:513:PRO:HG3	1:A:537:SER:HA	1.97	0.45
1:B:592:MET:HE3	1:B:670:MET:SD	2.57	0.45
1:C:15:ILE:HD13	1:C:92:TYR:CD1	2.52	0.45
1:C:254:GLU:HB2	1:C:259:SER:HA	1.98	0.45
1:D:642:ARG:HB3	1:D:646:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD23	1:D:651:LEU:HA	1.86	0.45
1:A:276:LEU:CD2	1:A:341:ILE:HD13	2.47	0.45
1:A:376:GLN:HB2	1:A:378:LYS:HG3	1.99	0.45
1:B:313:ARG:NH1	1:B:313:ARG:CG	2.78	0.45
1:B:818:ASN:OD1	1:B:857:LEU:HD11	2.16	0.45
1:C:52:ILE:HD12	1:C:428:GLU:CG	2.46	0.45
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.46	0.45
1:C:405:LYS:O	1:C:690:GLY:HA2	2.16	0.45
1:D:50:PHE:HD2	1:D:54:GLY:O	2.00	0.45
1:D:297:GLU:O	1:D:298:LEU:HD23	2.16	0.45
1:D:642:ARG:NH2	1:D:646:HIS:NE2	2.65	0.45
1:D:658:ARG:HG3	1:D:658:ARG:NH1	2.31	0.45
1:D:775:ASN:CG	1:D:777:ILE:HD11	2.42	0.45
1:D:806:ARG:HB3	1:D:806:ARG:HH11	1.82	0.45
2:I:13:DG:O6	3:J:104:DG:O6	2.35	0.45
1:B:347:MET:CE	1:B:562:LEU:HD21	2.47	0.45
1:C:167:ALA:HA	1:C:176:ASP:OD1	2.17	0.45
1:C:553:MET:HE2	1:C:556:GLN:NE2	2.32	0.45
1:D:41:CYS:HB2	1:D:42:PRO:HD2	1.99	0.45
1:D:471:VAL:HB	1:D:472:PRO:CD	2.42	0.45
1:D:776:TYR:OH	1:D:854:ILE:HG22	2.17	0.45
1:A:347:MET:CB	1:A:558:ASN:HD21	2.22	0.44
1:A:412:LEU:HD22	1:A:415:LEU:CD1	2.46	0.44
1:A:725:LEU:HD12	1:A:725:LEU:N	2.32	0.44
1:C:61:LEU:HD23	1:C:62:PHE:N	2.32	0.44
1:C:295:GLU:HA	1:C:300:VAL:H	1.82	0.44
1:C:302:LYS:HD2	1:C:323:TYR:CD2	2.52	0.44
1:C:314:GLU:O	1:C:315:SER:C	2.60	0.44
1:C:431:ALA:HB1	1:C:454:TYR:CE2	2.52	0.44
1:D:44:SER:O	1:D:46:ALA:N	2.49	0.44
1:D:406:TYR:HE2	1:D:647:TRP:CE2	2.36	0.44
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.52	0.44
1:D:484:GLU:HG2	1:D:488:TYR:CE1	2.52	0.44
1:D:705:LYS:H	1:D:705:LYS:HG2	1.65	0.44
1:D:818:ASN:C	1:D:820:ASP:N	2.75	0.44
1:A:218:VAL:HG13	1:A:223:ILE:HD12	2.00	0.44
1:A:321:ILE:O	1:A:325:ILE:HG13	2.16	0.44
1:A:658:ARG:HG3	1:A:658:ARG:NH1	2.32	0.44
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.33	0.44
1:C:457:SER:O	1:C:459:ASN:N	2.50	0.44
1:C:525:GLU:N	1:C:525:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:ASN:ND2	1:C:572:ASN:C	2.76	0.44
1:D:116:GLU:CG	1:D:324:ASN:HD22	2.22	0.44
1:D:198:LEU:O	1:D:201:TYR:N	2.51	0.44
3:L:114:DA:C2	3:L:115:DA:N1	2.85	0.44
1:A:499:ILE:O	1:A:503:LEU:HG	2.17	0.44
1:A:731:GLU:HA	1:A:734:LYS:HG2	2.00	0.44
1:B:85:MET:HE3	1:B:90:LEU:HB3	2.00	0.44
1:B:352:LYS:HB2	5:B:923:HOH:O	2.18	0.44
1:B:750:ARG:HH11	1:B:754:GLN:NE2	2.15	0.44
1:C:313:ARG:HG2	1:C:320:TYR:CE1	2.53	0.44
1:C:654:PHE:CD1	1:C:654:PHE:C	2.96	0.44
1:C:779:ILE:HD11	1:C:866:MET:HE1	1.98	0.44
1:D:504:HIS:C	1:D:504:HIS:CD2	2.95	0.44
1:D:727:ILE:HG23	1:D:730:LEU:CD1	2.39	0.44
1:D:758:GLU:CG	1:D:759:SER:H	2.29	0.44
3:L:114:DA:H2''	3:L:115:DA:OP2	2.18	0.44
1:A:44:SER:O	1:A:46:ALA:N	2.51	0.44
1:A:489:MET:HE2	1:A:556:GLN:HE22	1.82	0.44
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.48	0.44
1:B:503:LEU:HD12	1:B:542:LEU:CG	2.44	0.44
1:C:453:VAL:HG23	1:C:454:TYR:CD2	2.52	0.44
1:D:499:ILE:HD12	1:D:545:ALA:HB2	2.00	0.44
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.82	0.44
1:D:530:ILE:C	1:D:532:LYS:H	2.26	0.44
1:B:85:MET:HE2	1:B:370:PHE:CG	2.53	0.44
1:B:397:LYS:HB3	1:B:620:GLY:H	1.83	0.44
1:B:523:SER:N	1:B:526:ILE:HD12	2.30	0.44
1:B:636:VAL:HG13	1:B:640:LYS:CE	2.44	0.44
1:C:218:VAL:HG23	1:C:222:ALA:HB3	1.99	0.44
1:C:291:ASP:OD1	1:C:301:GLY:HA3	2.18	0.44
1:C:800:LYS:HA	2:I:11:DC:O3'	2.16	0.44
1:C:831:TYR:CD2	1:C:850:SER:HA	2.52	0.44
1:D:7:THR:HG21	1:D:267:GLY:O	2.18	0.44
1:D:140:ASP:OD1	1:D:141:SER:N	2.50	0.44
1:D:556:GLN:HE21	1:D:557:ILE:HG12	1.82	0.44
1:A:138:HIS:HD2	1:A:201:TYR:OH	1.99	0.44
1:A:443:ILE:HD13	1:A:595:GLN:HB2	2.00	0.44
1:A:480:ASN:O	1:A:483:LYS:HG2	2.17	0.44
1:A:492:ALA:HB3	1:A:549:GLU:HB2	2.00	0.44
1:A:546:GLN:O	1:A:550:VAL:HG13	2.17	0.44
1:A:787:ASN:O	1:A:790:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:TYR:CD1	1:B:92:TYR:C	2.95	0.44
1:B:355:ILE:O	1:B:358:VAL:HG13	2.18	0.44
1:B:644:THR:HG21	1:C:77:ASP:OD2	2.18	0.44
1:B:797:PRO:HG3	1:B:806:ARG:HH12	1.83	0.44
1:B:839:ASN:HA	1:B:840:PRO:HD3	1.85	0.44
1:B:871:LEU:O	1:B:875:THR:HG23	2.18	0.44
1:C:163:SER:CB	1:C:166:ILE:HG13	2.48	0.44
1:C:252:VAL:O	1:C:252:VAL:HG12	2.17	0.44
1:C:489:MET:C	1:C:491:ALA:H	2.24	0.44
1:D:42:PRO:HG2	1:D:45:GLN:HB2	2.00	0.44
1:D:445:ALA:HA	1:D:673:TYR:CE1	2.53	0.44
1:D:862:VAL:C	1:D:864:HIS:H	2.26	0.44
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.82	0.44
1:A:490:LEU:O	1:A:494:ARG:HB3	2.17	0.44
1:B:298:LEU:CD1	1:B:333:GLN:HB2	2.48	0.44
1:C:34:LYS:HD3	1:C:61:LEU:CD2	2.48	0.44
1:C:189:MET:HB3	1:C:191:PHE:HE1	1.82	0.44
1:C:432:GLY:CA	1:C:462:MET:HE2	2.47	0.44
1:C:481:GLN:HB3	1:C:559:ARG:NH1	2.32	0.44
1:D:466:ASP:CG	1:D:467:ARG:N	2.75	0.44
1:A:483:LYS:HB2	1:A:483:LYS:NZ	2.33	0.44
1:A:656:ARG:HA	1:A:660:GLU:CG	2.48	0.44
1:C:109:ARG:NH1	1:C:140:ASP:OD2	2.51	0.44
1:C:133:ILE:HD13	1:C:226:VAL:HG22	2.00	0.44
1:C:399:PRO:HB3	1:C:619:TYR:HB2	1.99	0.44
1:C:725:LEU:HD11	1:C:750:ARG:HB2	1.99	0.44
1:D:133:ILE:HD11	1:D:229:ARG:CG	2.35	0.44
1:D:149:PHE:N	1:D:149:PHE:CD1	2.86	0.44
1:D:205:TRP:C	1:D:207:GLN:N	2.74	0.44
1:D:419:ILE:HD13	1:D:589:PHE:HB3	2.00	0.44
1:D:570:LEU:HA	1:D:570:LEU:HD23	1.81	0.44
1:D:769:LYS:O	1:D:770:GLU:C	2.61	0.44
1:A:113:PHE:CE1	1:A:218:VAL:HG21	2.53	0.44
1:B:123:PHE:HA	1:B:124:PRO:HD3	1.86	0.44
1:B:171:GLN:NE2	1:B:303:LEU:HD13	2.20	0.44
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.53	0.44
1:C:33:TYR:OH	1:C:95:ASP:OD2	2.18	0.44
1:C:249:ARG:HG3	1:C:249:ARG:NH1	2.31	0.44
1:D:578:TYR:CD1	1:D:578:TYR:C	2.95	0.44
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.53	0.44
3:J:114:DA:H2"	3:J:115:DA:H5"	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:5:DG:N3	2:K:6:DA:O4'	2.51	0.44
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.53	0.43
1:B:152:LEU:CD1	1:B:190:PRO:HB2	2.44	0.43
1:B:351:ALA:O	1:B:352:LYS:HB2	2.18	0.43
1:B:491:ALA:HB3	1:B:519:ARG:O	2.18	0.43
1:B:818:ASN:CG	1:B:857:LEU:HD11	2.43	0.43
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.53	0.43
1:C:472:PRO:C	1:C:475:ILE:HG22	2.43	0.43
1:C:493:GLN:C	1:C:495:ASN:H	2.26	0.43
1:C:530:ILE:C	1:C:532:LYS:N	2.76	0.43
1:D:491:ALA:CB	1:D:520:PHE:HA	2.49	0.43
1:D:832:VAL:HG22	1:D:847:ALA:CB	2.48	0.43
1:A:612:GLU:OE1	1:A:612:GLU:N	2.43	0.43
1:C:461:MET:HE2	1:C:461:MET:N	2.33	0.43
1:D:126:PRO:HB2	1:D:224:PRO:HB2	2.00	0.43
1:D:182:ILE:O	1:D:186:ILE:HG23	2.18	0.43
1:D:268:ILE:HG22	1:D:269:SER:N	2.31	0.43
1:D:453:VAL:HG23	1:D:454:TYR:CG	2.53	0.43
1:D:622:THR:CG2	1:D:623:ASP:N	2.81	0.43
1:D:782:VAL:HG12	1:D:783:SER:N	2.33	0.43
1:D:892:GLU:O	1:D:894:LYS:HE3	2.18	0.43
1:A:51:ASP:OD2	1:A:53:TYR:N	2.46	0.43
1:A:503:LEU:HD21	1:A:539:ASN:OD1	2.18	0.43
1:A:627:VAL:HG12	1:A:628:SER:N	2.33	0.43
1:A:767:PHE:CD1	1:A:767:PHE:C	2.97	0.43
1:A:776:TYR:OH	1:A:853:GLU:HG3	2.17	0.43
1:B:582:ASN:O	1:B:586:ILE:HG13	2.19	0.43
1:C:431:ALA:HB1	1:C:454:TYR:CZ	2.53	0.43
1:C:611:THR:CG2	1:C:612:GLU:N	2.81	0.43
1:D:86:ASP:OD2	1:D:86:ASP:N	2.43	0.43
1:D:122:GLY:HA3	1:D:826:GLU:HB2	2.00	0.43
1:D:290:LEU:O	1:D:290:LEU:HD23	2.19	0.43
1:D:581:ARG:HG2	1:D:581:ARG:HH11	1.83	0.43
1:B:466:ASP:CG	1:B:467:ARG:H	2.25	0.43
1:B:727:ILE:HD13	1:B:749:ILE:HD13	2.00	0.43
1:C:6:LEU:HD11	1:C:26:GLU:HG2	2.00	0.43
1:C:65:MET:HB3	1:C:88:PHE:CD2	2.53	0.43
1:D:126:PRO:C	1:D:128:GLN:N	2.74	0.43
1:D:152:LEU:HD12	1:D:152:LEU:N	2.32	0.43
1:D:206:GLN:NE2	1:D:241:ARG:HB3	2.33	0.43
1:D:595:GLN:HE21	1:D:595:GLN:HB3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:ARG:HH11	1:D:599:ARG:CB	2.29	0.43
1:D:728:MET:HE2	1:D:728:MET:HA	2.00	0.43
1:D:749:ILE:O	1:D:750:ARG:C	2.60	0.43
1:A:64:ASN:C	1:A:64:ASN:ND2	2.76	0.43
1:A:65:MET:HB3	1:A:88:PHE:CD1	2.53	0.43
1:A:97:TYR:O	1:A:352:LYS:CE	2.61	0.43
1:A:128:GLN:O	1:A:129:ALA:C	2.62	0.43
1:A:492:ALA:CB	1:A:549:GLU:HB2	2.49	0.43
1:A:731:GLU:CG	1:A:879:PRO:HB3	2.40	0.43
1:A:738:PRO:HG2	1:A:741:VAL:CB	2.48	0.43
1:B:19:TYR:HE1	1:B:29:ARG:HG2	1.82	0.43
1:B:129:ALA:HA	1:B:225:TYR:CE1	2.54	0.43
1:B:150:ASP:OD2	1:B:188:TYR:OH	2.24	0.43
1:B:391:TYR:HB2	1:B:392:PRO:HD2	2.00	0.43
1:B:503:LEU:HD23	1:B:506:PRO:HD3	2.00	0.43
1:B:541:MET:O	1:B:545:ALA:HB2	2.19	0.43
1:B:898:PHE:HE2	1:D:654:PHE:HB2	1.82	0.43
1:C:425:ILE:HG23	1:C:463:TYR:CE2	2.54	0.43
1:C:502:ALA:HB1	1:C:533:LEU:CD1	2.41	0.43
1:D:182:ILE:HD12	1:D:329:TYR:CG	2.53	0.43
1:D:252:VAL:HG23	1:D:252:VAL:O	2.19	0.43
1:D:338:ARG:HD2	1:D:340:PHE:CZ	2.52	0.43
3:J:107:DG:H2''	3:J:108:DT:C5'	2.48	0.43
1:A:547:ARG:O	1:A:550:VAL:HG22	2.18	0.43
1:B:455:SER:HA	1:B:675:ASN:O	2.18	0.43
1:B:634:ASP:C	1:B:636:VAL:H	2.25	0.43
1:C:128:GLN:O	1:C:129:ALA:C	2.62	0.43
1:C:154:SER:C	1:C:156:TYR:N	2.76	0.43
1:C:455:SER:OG	1:C:676:ASN:ND2	2.51	0.43
1:D:199:MET:O	1:D:203:ASN:HB2	2.18	0.43
1:D:319:ARG:O	1:D:323:TYR:N	2.48	0.43
1:D:440:HIS:NE2	1:D:444:ASN:ND2	2.66	0.43
1:D:733:GLN:HE21	1:D:733:GLN:CA	2.26	0.43
1:A:49:TYR:CE1	1:A:59:ARG:HD3	2.54	0.43
1:A:73:LYS:HA	1:A:76:GLU:OE2	2.18	0.43
1:A:410:PHE:CD1	1:A:410:PHE:N	2.87	0.43
1:A:833:LEU:HD13	1:A:866:MET:HE2	2.01	0.43
1:B:433:THR:O	1:B:462:MET:HE2	2.18	0.43
1:B:863:LEU:HD12	1:B:866:MET:HE3	2.00	0.43
1:B:875:THR:O	1:B:879:PRO:HG3	2.18	0.43
1:D:194:GLU:O	1:D:198:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ARG:HG2	1:D:246:ARG:HE	1.84	0.43
1:D:327:ALA:O	1:D:328:VAL:C	2.62	0.43
1:D:440:HIS:HA	1:D:443:ILE:HD12	2.01	0.43
1:D:662:ALA:HA	1:D:665:ARG:NH1	2.33	0.43
1:D:667:PHE:HD1	1:D:681:MET:O	2.01	0.43
1:D:677:LYS:HE2	5:D:924:HOH:O	2.18	0.43
1:D:731:GLU:O	1:D:732:THR:C	2.60	0.43
1:D:756:GLY:O	1:D:757:GLU:C	2.62	0.43
1:A:51:ASP:OD2	1:A:51:ASP:C	2.62	0.43
1:A:452:ASP:OD1	1:A:453:VAL:HG23	2.18	0.43
1:A:504:HIS:C	1:A:506:PRO:HD3	2.44	0.43
1:A:552:GLY:O	1:A:555:ALA:N	2.51	0.43
1:A:790:LYS:HG2	1:A:791:TYR:CE1	2.53	0.43
1:B:301:GLY:O	1:B:330:ARG:NE	2.46	0.43
1:B:538:LEU:HD22	1:B:542:LEU:CD2	2.49	0.43
1:C:362:ILE:HG12	2:I:2:DG:C5'	2.49	0.43
1:C:486:LYS:HG2	1:C:556:GLN:HG3	2.01	0.43
1:C:560:LYS:HE2	1:C:561:LEU:HD12	2.01	0.43
1:C:565:SER:HA	2:I:2:DG:N2	2.33	0.43
1:C:742:GLN:O	1:C:746:LYS:HB2	2.18	0.43
1:D:605:LEU:HD11	1:D:659:MET:CE	2.49	0.43
1:D:732:THR:C	1:D:734:LYS:H	2.27	0.43
1:D:766:GLU:C	1:D:766:GLU:OE1	2.62	0.43
3:J:101:DG:H2''	3:J:102:DC:C6	2.54	0.43
1:A:392:PRO:HG2	1:A:584:THR:HG23	2.00	0.43
1:A:438:PRO:O	1:A:441:ASP:HB2	2.18	0.43
1:A:455:SER:HA	1:A:675:ASN:O	2.19	0.43
1:A:514:LEU:O	1:A:516:VAL:N	2.50	0.43
1:A:537:SER:O	1:A:540:GLU:N	2.51	0.43
1:B:173:GLN:HE21	1:B:173:GLN:HB2	1.53	0.43
1:B:206:GLN:HE22	1:B:246:ARG:NH2	2.17	0.43
1:B:236:GLU:O	1:B:240:LYS:HG3	2.18	0.43
1:B:752:MET:HE3	1:B:889:LEU:CD1	2.47	0.43
1:C:5:TYR:HE1	1:C:101:ILE:CD1	2.32	0.43
1:C:475:ILE:HG23	1:C:476:THR:H	1.84	0.43
1:C:503:LEU:HD21	1:C:538:LEU:HD22	1.99	0.43
1:C:824:VAL:HG22	1:C:849:PRO:HD3	2.00	0.43
1:D:153:ASN:HA	1:D:158:ASN:HD21	1.83	0.43
1:D:332:LEU:N	1:D:332:LEU:CD1	2.82	0.43
1:D:439:LEU:HD12	1:D:439:LEU:HA	1.89	0.43
1:D:524:ASP:HA	1:D:527:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:GLN:O	1:D:734:LYS:C	2.61	0.43
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.19	0.43
1:A:828:GLU:C	1:A:829:LYS:HE3	2.44	0.43
1:B:251:LYS:HE3	1:B:262:ILE:HD11	2.01	0.43
1:C:65:MET:HE1	1:C:88:PHE:HB3	1.99	0.43
1:C:159:VAL:CG1	1:C:160:GLU:H	2.23	0.43
1:C:234:PHE:HB3	1:C:238:THR:OG1	2.19	0.43
1:C:243:SER:HB2	1:C:248:THR:HG22	2.01	0.43
1:C:314:GLU:HG2	1:C:315:SER:H	1.83	0.43
1:C:553:MET:O	1:C:554:THR:C	2.61	0.43
1:C:572:ASN:HD21	1:C:574:TRP:HB2	1.83	0.43
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.91	0.43
1:D:48:LYS:HE3	1:D:49:TYR:CZ	2.53	0.43
1:D:112:ASN:O	1:D:328:VAL:HG13	2.18	0.43
1:D:170:LEU:HG	1:D:171:GLN:H	1.82	0.43
1:D:499:ILE:HG21	1:D:541:MET:C	2.44	0.43
1:A:197:LEU:HD23	1:A:197:LEU:C	2.44	0.42
1:A:708:TYR:CE2	1:A:726:LYS:HE2	2.53	0.42
1:A:786:ASN:HD22	1:A:786:ASN:N	2.17	0.42
1:A:793:VAL:O	1:A:793:VAL:HG12	2.19	0.42
1:B:365:TRP:CD2	1:B:566:LEU:HD13	2.53	0.42
1:C:667:PHE:HB3	1:C:679:HIS:HE1	1.83	0.42
1:C:745:LEU:HD23	1:C:745:LEU:HA	1.85	0.42
1:D:147:TYR:N	1:D:147:TYR:CD1	2.87	0.42
1:D:202:LEU:HD21	1:D:241:ARG:NH1	2.33	0.42
1:D:362:ILE:HD11	1:D:575:PHE:HA	2.01	0.42
1:D:776:TYR:C	1:D:778:SER:N	2.76	0.42
1:D:830:VAL:HG22	1:D:847:ALA:HB1	2.01	0.42
1:B:197:LEU:HD23	1:B:197:LEU:O	2.18	0.42
1:B:271:LEU:HB3	1:B:276:LEU:HD11	2.00	0.42
1:B:641:PHE:HA	1:B:646:HIS:HD2	1.84	0.42
1:B:658:ARG:HH11	1:B:658:ARG:HG3	1.83	0.42
1:B:873:GLU:HA	1:B:877:ILE:CG1	2.49	0.42
1:C:806:ARG:HG2	1:C:806:ARG:NH1	2.25	0.42
1:A:273:TYR:HE1	1:A:335:ASP:OD2	2.02	0.42
1:A:497:GLU:HA	1:A:497:GLU:OE2	2.20	0.42
1:B:13:ASP:OD2	1:B:66:ARG:HB2	2.19	0.42
1:B:178:VAL:HA	1:B:326:ILE:HD11	2.01	0.42
1:B:386:HIS:HB2	1:B:573:VAL:HG22	2.01	0.42
1:C:269:SER:HB3	1:C:356:GLN:HG3	2.01	0.42
1:C:530:ILE:C	1:C:532:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ARG:HA	1:C:660:GLU:HG3	2.01	0.42
1:D:48:LYS:HE3	1:D:49:TYR:OH	2.19	0.42
1:D:234:PHE:CD2	1:D:238:THR:HG21	2.54	0.42
1:D:376:GLN:HB2	1:D:378:LYS:HG3	2.01	0.42
1:A:150:ASP:OD1	1:A:317:HIS:CE1	2.73	0.42
1:A:416:TYR:N	1:A:416:TYR:CD2	2.87	0.42
1:A:784:SER:OG	1:A:829:LYS:HE2	2.19	0.42
1:A:785:ALA:HB1	1:A:808:ILE:CD1	2.48	0.42
1:B:362:ILE:HG12	2:G:2:DG:H5'	2.02	0.42
1:B:779:ILE:HD12	1:B:871:LEU:CD2	2.48	0.42
1:C:36:SER:HB3	1:C:59:ARG:HD2	2.01	0.42
1:C:132:PRO:HB3	1:C:194:GLU:OE1	2.19	0.42
1:C:441:ASP:HB3	1:C:447:ALA:HB2	2.00	0.42
1:C:896:SER:C	1:C:897:LEU:HD12	2.44	0.42
1:D:126:PRO:C	1:D:128:GLN:H	2.26	0.42
1:D:406:TYR:HB3	1:D:629:ALA:HB3	2.02	0.42
1:D:660:GLU:CB	1:D:661:PRO:HD3	2.48	0.42
1:A:212:ILE:HD13	1:A:269:SER:HB2	2.02	0.42
1:A:415:LEU:HG	1:A:419:ILE:HD11	2.02	0.42
1:B:416:TYR:CD2	4:B:907:DTP:C2'	3.00	0.42
1:B:643:ASP:HA	1:B:693:LEU:HD23	2.01	0.42
1:C:542:LEU:C	1:C:544:ARG:N	2.74	0.42
1:C:641:PHE:CE2	1:C:647:TRP:HA	2.54	0.42
1:D:187:ILE:O	1:D:187:ILE:HG22	2.19	0.42
1:D:199:MET:HB3	1:D:234:PHE:HE2	1.84	0.42
1:D:290:LEU:O	1:D:294:SER:CB	2.68	0.42
1:D:362:ILE:HD11	1:D:575:PHE:CA	2.49	0.42
1:D:401:PRO:HG3	1:D:703:THR:O	2.20	0.42
1:D:499:ILE:CD1	1:D:545:ALA:HB2	2.49	0.42
1:D:734:LYS:HG3	1:D:735:SER:H	1.84	0.42
1:D:856:ASP:HA	1:D:859:LYS:HB3	2.00	0.42
3:L:109:DC:OP1	3:L:109:DC:H4'	2.18	0.42
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.34	0.42
1:A:296:PHE:C	1:A:296:PHE:CD2	2.97	0.42
1:A:605:LEU:HA	1:A:608:VAL:HG22	2.00	0.42
1:A:785:ALA:HB2	1:A:808:ILE:HD11	2.01	0.42
1:B:154:SER:C	1:B:156:TYR:H	2.27	0.42
1:B:195:LYS:HG2	1:B:234:PHE:CZ	2.54	0.42
1:B:625:ILE:HG12	1:B:683:MET:HE2	2.02	0.42
1:C:62:PHE:HE2	1:C:71:TRP:HB2	1.84	0.42
1:C:65:MET:H	1:C:65:MET:HG2	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ARG:HA	1:C:660:GLU:CG	2.50	0.42
1:C:680:LEU:HA	1:C:682:PHE:CZ	2.54	0.42
1:D:440:HIS:CE1	1:D:444:ASN:ND2	2.83	0.42
1:D:741:VAL:O	1:D:744:ALA:N	2.52	0.42
2:E:7:DA:H4'	2:E:8:DT:OP1	2.19	0.42
1:A:68:ALA:O	1:A:72:ILE:HG13	2.20	0.42
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.55	0.42
1:A:656:ARG:HA	1:A:660:GLU:HG3	2.02	0.42
1:A:682:PHE:HA	5:A:924:HOH:O	2.19	0.42
1:A:844:LYS:HB3	1:A:844:LYS:HE2	1.86	0.42
1:B:524:ASP:O	1:B:526:ILE:N	2.52	0.42
1:B:649:ASP:OD2	1:B:649:ASP:N	2.52	0.42
1:C:362:ILE:HD13	1:C:362:ILE:HA	1.90	0.42
1:C:703:THR:OG1	1:C:707:ARG:HB2	2.20	0.42
1:C:876:PHE:O	1:C:879:PRO:HG2	2.20	0.42
1:D:62:PHE:N	1:D:62:PHE:CD1	2.87	0.42
1:D:161:GLU:HG2	1:D:162:TRP:H	1.85	0.42
1:D:401:PRO:O	1:D:402:ASN:HB2	2.19	0.42
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.33	0.42
1:A:518:TYR:CD2	1:A:545:ALA:HB2	2.55	0.42
1:A:572:ASN:C	1:A:572:ASN:ND2	2.77	0.42
1:B:101:ILE:HG21	1:B:349:TYR:CG	2.55	0.42
1:B:525:GLU:HG2	1:B:525:GLU:O	2.19	0.42
1:C:597:ILE:HB	1:C:667:PHE:CZ	2.54	0.42
1:C:768:GLU:HG2	1:C:872:LEU:HD21	2.02	0.42
1:D:15:ILE:HD11	1:D:92:TYR:CE2	2.54	0.42
1:D:122:GLY:O	1:D:123:PHE:C	2.63	0.42
1:D:202:LEU:O	1:D:205:TRP:HB3	2.20	0.42
1:D:254:GLU:HA	1:D:259:SER:HA	2.00	0.42
1:D:329:TYR:O	1:D:333:GLN:HG3	2.20	0.42
1:A:396:VAL:HG12	1:A:705:LYS:HG2	2.01	0.42
1:A:548:THR:O	1:A:549:GLU:C	2.63	0.42
1:A:550:VAL:HG23	1:A:551:ALA:N	2.35	0.42
1:B:216:TRP:HZ2	1:B:293:ILE:HG13	1.84	0.42
1:B:395:PHE:HB2	1:B:591:GLN:CG	2.50	0.42
1:B:506:PRO:HB3	1:B:538:LEU:CD1	2.50	0.42
1:B:770:GLU:O	1:B:773:GLN:HG2	2.19	0.42
1:C:233:ILE:HG22	1:C:234:PHE:CE2	2.55	0.42
1:C:407:VAL:HA	1:C:627:VAL:O	2.20	0.42
1:C:426:SER:OG	1:C:427:PRO:HD2	2.20	0.42
1:C:681:MET:C	1:C:682:PHE:CD1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:SER:O	1:C:852:THR:HG23	2.19	0.42
1:D:137:THR:O	1:D:328:VAL:HG21	2.20	0.42
1:D:739:LYS:CE	1:D:743:LYS:HD2	2.50	0.42
1:A:118:THR:N	1:A:134:ASP:OD2	2.52	0.42
1:A:508:LEU:N	1:A:508:LEU:CD2	2.82	0.42
1:A:606:ASN:OD1	1:A:616:PHE:HE1	2.02	0.42
1:A:787:ASN:HB3	1:A:790:LYS:HB3	2.00	0.42
1:A:810:THR:OG1	1:A:843:ASP:HB2	2.20	0.42
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.55	0.42
1:B:632:ILE:HA	1:B:632:ILE:HD13	1.83	0.42
1:B:634:ASP:C	1:B:636:VAL:N	2.77	0.42
1:B:727:ILE:HD13	1:B:749:ILE:CD1	2.49	0.42
1:C:510:VAL:O	1:C:510:VAL:HG12	2.19	0.42
1:D:51:ASP:OD1	1:D:51:ASP:C	2.62	0.42
1:D:253:ILE:HG23	1:D:260:ARG:NH1	2.35	0.42
1:D:296:PHE:CD1	1:D:296:PHE:C	2.97	0.42
1:D:380:ILE:HB	1:D:576:ARG:HD3	2.02	0.42
1:D:430:ILE:CG2	1:D:461:MET:HE2	2.50	0.42
1:D:445:ALA:HB2	1:D:596:TRP:CZ3	2.54	0.42
1:D:449:ARG:HH11	1:D:452:ASP:HB3	1.76	0.42
1:D:492:ALA:HA	1:D:495:ASN:HB3	2.00	0.42
1:D:633:ILE:HD13	1:D:633:ILE:HA	1.90	0.42
2:E:15:DC:O2	3:F:104:DG:N2	2.53	0.42
1:A:171:GLN:HE22	1:A:319:ARG:CZ	2.33	0.41
1:B:681:MET:HA	1:B:681:MET:HE2	2.02	0.41
1:C:402:ASN:HA	1:C:886:ALA:O	2.19	0.41
1:C:423:VAL:HB	1:C:425:ILE:HG13	2.02	0.41
1:D:734:LYS:HE2	1:D:734:LYS:HB2	1.89	0.41
1:D:741:VAL:C	1:D:743:LYS:N	2.78	0.41
1:A:199:MET:HA	1:A:199:MET:HE3	2.02	0.41
1:B:45:GLN:O	1:B:47:THR:HG22	2.20	0.41
1:B:185:LYS:H	1:B:185:LYS:HG2	1.62	0.41
1:B:625:ILE:HG12	1:B:683:MET:CE	2.50	0.41
1:B:678:GLN:HG2	1:B:680:LEU:HG	2.02	0.41
1:C:299:ASN:O	1:C:300:VAL:HB	2.20	0.41
1:C:420:ILE:HG12	1:C:586:ILE:HD11	2.01	0.41
1:C:727:ILE:CG2	1:C:730:LEU:HB2	2.51	0.41
1:C:887:ALA:O	1:C:888:LYS:HB2	2.20	0.41
1:D:456:CYS:HB2	1:D:674:MET:HE3	2.01	0.41
1:D:495:ASN:HD22	1:D:495:ASN:C	2.20	0.41
1:D:642:ARG:HG2	1:D:643:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:777:ILE:HD12	1:D:778:SER:H	1.81	0.41
1:A:75:MET:HE1	1:A:80:LEU:HB3	2.03	0.41
1:A:405:LYS:HA	1:A:698:ILE:O	2.21	0.41
1:B:164:ILE:N	1:B:164:ILE:CD1	2.81	0.41
1:C:425:ILE:HA	1:C:463:TYR:CD2	2.55	0.41
1:C:682:PHE:CD1	1:C:682:PHE:N	2.86	0.41
1:D:97:TYR:HB3	1:D:101:ILE:CD1	2.37	0.41
1:D:277:TYR:O	1:D:281:SER:HB2	2.19	0.41
1:D:704:GLY:O	1:D:705:LYS:C	2.63	0.41
1:D:788:ILE:HD11	1:D:809:LEU:HD23	2.02	0.41
2:G:16:DG:H2''	2:G:17:DC:H5'	2.01	0.41
1:A:616:PHE:HE2	1:A:631:LYS:HB3	1.86	0.41
1:B:517:ASP:O	1:B:519:ARG:N	2.54	0.41
1:B:530:ILE:C	1:B:532:LYS:N	2.77	0.41
1:C:308:PRO:HG3	1:C:311:LYS:HE3	2.01	0.41
1:C:415:LEU:HD22	1:C:623:ASP:HB3	2.03	0.41
1:C:452:ASP:O	1:C:452:ASP:OD2	2.38	0.41
1:C:499:ILE:CG2	1:C:541:MET:HE2	2.50	0.41
1:C:500:LYS:HA	1:C:503:LEU:HD12	2.01	0.41
1:C:561:LEU:CD1	1:C:561:LEU:H	2.33	0.41
1:D:93:LEU:HD23	1:D:352:LYS:C	2.45	0.41
1:D:362:ILE:HD13	1:D:575:PHE:CD1	2.55	0.41
1:D:398:GLU:HA	1:D:705:LYS:CE	2.51	0.41
1:D:596:TRP:NE1	1:D:670:MET:HB2	2.35	0.41
1:D:708:TYR:CD2	1:D:708:TYR:C	2.99	0.41
1:D:720:TYR:CD2	1:D:724:LYS:HG2	2.56	0.41
1:D:779:ILE:HG22	1:D:871:LEU:CD2	2.50	0.41
1:D:860:ASP:O	1:D:864:HIS:HB2	2.21	0.41
3:L:105:DC:H2'	3:L:106:DT:C6	2.55	0.41
1:A:518:TYR:O	1:A:520:PHE:N	2.54	0.41
1:A:701:PHE:CD1	1:A:701:PHE:C	2.99	0.41
1:A:711:ASN:ND2	1:A:723:PRO:HB2	2.36	0.41
1:A:786:ASN:O	1:A:805:ILE:HD11	2.20	0.41
1:B:171:GLN:HE22	1:B:303:LEU:CD1	2.23	0.41
1:B:500:LYS:HA	1:B:542:LEU:HD11	2.03	0.41
1:C:217:ASN:HD22	1:C:274:ILE:HD13	1.84	0.41
1:C:283:THR:O	1:C:283:THR:HG23	2.20	0.41
1:C:397:LYS:O	1:C:399:PRO:HD3	2.21	0.41
1:C:592:MET:CE	1:C:670:MET:SD	3.08	0.41
1:D:227:TYR:CG	1:D:263:ILE:HD13	2.54	0.41
1:D:283:THR:O	1:D:285:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:ILE:HG23	1:D:824:VAL:HG11	2.02	0.41
1:D:815:ILE:HD12	1:D:815:ILE:O	2.21	0.41
2:G:4:CTG:O6	2:G:4:CTG:H2'	2.21	0.41
3:J:104:DG:H2''	3:J:105:DC:C6	2.56	0.41
3:L:108:DT:C1'	3:L:109:DC:H5''	2.51	0.41
1:A:338:ARG:HB3	1:A:340:PHE:CZ	2.55	0.41
1:A:518:TYR:OH	1:A:541:MET:HB3	2.21	0.41
1:B:749:ILE:O	1:B:753:LEU:CD1	2.63	0.41
1:C:193:ASN:OD1	1:C:196:GLU:CG	2.67	0.41
1:C:505:ASN:O	1:C:506:PRO:C	2.61	0.41
1:C:518:TYR:HA	1:C:522:PHE:HE1	1.84	0.41
1:D:179:PRO:HB2	1:D:182:ILE:HG21	2.02	0.41
1:D:305:TYR:HD2	1:D:305:TYR:O	2.02	0.41
1:D:411:ASP:O	1:D:683:MET:HA	2.21	0.41
1:D:771:PHE:CE2	1:D:872:LEU:HD13	2.56	0.41
3:L:108:DT:H2''	3:L:109:DC:O5'	2.15	0.41
1:A:183:ILE:HD12	1:A:183:ILE:HA	1.88	0.41
1:A:202:LEU:CD1	1:A:242:LEU:HD13	2.51	0.41
1:A:249:ARG:NH2	1:A:251:LYS:NZ	2.57	0.41
1:B:423:VAL:O	1:B:424:ASN:CB	2.69	0.41
1:D:221:PHE:O	1:D:222:ALA:C	2.63	0.41
1:D:477:LYS:O	1:D:481:GLN:HG3	2.20	0.41
1:A:92:TYR:CD1	1:A:92:TYR:C	2.98	0.41
1:A:285:GLN:OE1	1:A:296:PHE:CE1	2.74	0.41
1:A:634:ASP:C	1:A:636:VAL:N	2.78	0.41
1:A:642:ARG:HB2	1:A:646:HIS:CD2	2.55	0.41
1:B:109:ARG:NH1	1:B:142:ILE:HD12	2.36	0.41
1:B:280:PHE:HB2	1:B:340:PHE:CE1	2.55	0.41
1:B:626:TYR:CD1	1:B:626:TYR:N	2.89	0.41
1:C:166:ILE:HB	1:C:318:GLN:OE1	2.20	0.41
1:D:136:ILE:HD11	1:D:201:TYR:CZ	2.55	0.41
1:D:461:MET:HB3	1:D:463:TYR:CE1	2.56	0.41
1:D:500:LYS:C	1:D:502:ALA:N	2.77	0.41
1:D:692:PRO:CD	1:D:754:GLN:HA	2.50	0.41
1:D:710:LEU:HD13	1:D:712:VAL:HG22	2.02	0.41
1:D:831:TYR:CD1	1:D:848:TRP:CZ3	3.09	0.41
1:D:886:ALA:C	1:D:888:LYS:N	2.78	0.41
1:A:48:LYS:NZ	1:A:48:LYS:CB	2.84	0.41
1:A:170:LEU:HA	1:A:177:GLU:HG2	2.03	0.41
1:A:408:MET:SD	1:A:655:ALA:HB2	2.61	0.41
1:A:481:GLN:O	1:A:484:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TYR:OH	1:A:580:LEU:HD13	2.21	0.41
1:A:731:GLU:HA	1:A:734:LYS:CD	2.51	0.41
1:B:402:ASN:OD1	1:B:888:LYS:HE2	2.20	0.41
1:B:514:LEU:CD2	1:B:530:ILE:HG12	2.48	0.41
1:B:535:ALA:O	1:B:539:ASN:CG	2.64	0.41
1:B:738:PRO:HG3	1:B:780:ALA:C	2.46	0.41
1:C:486:LYS:CG	1:C:556:GLN:HG3	2.51	0.41
1:C:494:ARG:HG2	1:C:494:ARG:NH1	2.36	0.41
1:C:569:ALA:C	1:C:571:GLY:N	2.78	0.41
1:C:640:LYS:HE3	1:C:640:LYS:HB2	1.92	0.41
1:D:10:GLN:NE2	1:D:88:PHE:HD2	2.18	0.41
1:D:83:LEU:HB3	1:D:379:VAL:HG12	2.02	0.41
1:D:243:SER:C	1:D:245:HIS:N	2.79	0.41
1:D:257:TYR:CD1	1:D:257:TYR:N	2.89	0.41
1:D:423:VAL:O	1:D:424:ASN:CB	2.69	0.41
1:D:566:LEU:O	1:D:566:LEU:HG	2.19	0.41
1:D:731:GLU:HG2	2:K:7:DA:H5''	2.02	0.41
1:D:802:PRO:O	1:D:805:ILE:N	2.53	0.41
1:D:818:ASN:OD1	1:D:818:ASN:N	2.54	0.41
1:D:831:TYR:HD1	1:D:848:TRP:CZ3	2.38	0.41
2:G:16:DG:C1'	2:G:17:DC:H5''	2.49	0.41
2:I:14:DC:H2''	2:I:15:DC:H5'	2.00	0.41
3:J:107:DG:H1'	3:J:108:DT:H5''	2.03	0.41
1:A:480:ASN:O	1:A:481:GLN:C	2.63	0.41
1:A:629:ALA:O	1:A:630:ASP:C	2.64	0.41
1:A:741:VAL:CG1	1:A:745:LEU:HD22	2.51	0.41
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.84	0.41
1:B:497:GLU:HA	1:B:497:GLU:OE2	2.21	0.41
1:B:872:LEU:HD11	1:B:876:PHE:HD2	1.86	0.41
1:C:505:ASN:H	1:C:506:PRO:HD3	1.85	0.41
1:C:561:LEU:HD12	1:C:561:LEU:N	2.36	0.41
1:C:608:VAL:O	1:C:608:VAL:HG12	2.21	0.41
1:C:818:ASN:ND2	1:C:857:LEU:CD1	2.76	0.41
1:D:19:TYR:N	1:D:19:TYR:CD1	2.89	0.41
1:D:191:PHE:CE2	1:D:200:GLU:HG3	2.54	0.41
1:D:437:ALA:HB1	1:D:438:PRO:HD2	2.02	0.41
1:A:113:PHE:CE1	1:A:218:VAL:HG22	2.56	0.40
1:A:422:GLN:NE2	1:A:680:LEU:H	2.18	0.40
1:A:548:THR:O	1:A:551:ALA:HB3	2.20	0.40
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.80	0.40
1:B:286:PRO:HG2	1:B:292:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PRO:O	1:B:576:ARG:HD2	2.21	0.40
1:B:872:LEU:HD11	1:B:876:PHE:CD2	2.56	0.40
1:C:53:TYR:CD1	1:C:428:GLU:HB3	2.56	0.40
1:C:302:LYS:HD3	1:C:303:LEU:H	1.86	0.40
1:C:474:GLU:O	1:C:478:VAL:HG23	2.22	0.40
1:C:498:ILE:HG23	1:C:499:ILE:CD1	2.51	0.40
1:C:507:ASN:CB	1:C:531:LYS:O	2.68	0.40
1:C:533:LEU:CG	1:C:538:LEU:HG	2.51	0.40
1:C:558:ASN:N	1:C:558:ASN:HD22	2.17	0.40
1:C:580:LEU:HD12	1:C:580:LEU:HA	1.78	0.40
1:D:205:TRP:O	1:D:206:GLN:C	2.63	0.40
1:D:326:ILE:C	1:D:326:ILE:HD12	2.46	0.40
1:D:665:ARG:HB2	1:D:665:ARG:NH2	2.36	0.40
1:D:802:PRO:HD2	1:D:805:ILE:HG13	2.02	0.40
1:A:492:ALA:O	1:A:545:ALA:HB1	2.20	0.40
1:A:784:SER:CB	1:A:829:LYS:HE2	2.51	0.40
1:B:151:LEU:HD13	1:B:194:GLU:HA	2.03	0.40
1:B:205:TRP:HH2	1:B:213:LEU:CD2	2.34	0.40
1:C:193:ASN:HD21	1:C:195:LYS:HB2	1.85	0.40
1:C:302:LYS:CB	1:C:302:LYS:NZ	2.85	0.40
1:C:362:ILE:HD13	1:C:569:ALA:HB1	2.03	0.40
1:C:458:PRO:CG	1:C:592:MET:SD	3.10	0.40
1:C:507:ASN:ND2	1:C:508:LEU:N	2.67	0.40
1:D:105:HIS:CD2	1:D:106:THR:HG23	2.55	0.40
1:D:194:GLU:O	1:D:197:LEU:N	2.50	0.40
1:D:412:LEU:CD1	1:D:415:LEU:HD22	2.52	0.40
1:D:597:ILE:HD12	1:D:597:ILE:HA	1.88	0.40
1:D:758:GLU:CG	1:D:759:SER:N	2.85	0.40
1:D:791:TYR:HD2	1:D:801:CYS:CA	2.32	0.40
1:D:870:VAL:O	1:D:870:VAL:HG12	2.21	0.40
3:H:103:DG:H2"	3:H:104:DG:C8	2.56	0.40
1:A:250:VAL:HG12	1:A:263:ILE:HD12	2.03	0.40
1:A:493:GLN:O	1:A:496:GLY:N	2.52	0.40
1:A:497:GLU:C	1:A:499:ILE:H	2.28	0.40
1:B:52:ILE:HG13	1:B:53:TYR:CE1	2.56	0.40
1:B:166:ILE:O	1:B:169:LYS:HB2	2.21	0.40
1:B:219:GLU:OE1	1:B:262:ILE:HD12	2.21	0.40
1:B:389:GLN:HA	1:B:390:PRO:HD3	1.87	0.40
1:B:512:GLU:O	1:B:533:LEU:HD21	2.22	0.40
1:B:897:LEU:O	1:B:899:ASP:N	2.54	0.40
1:C:148:VAL:C	1:C:149:PHE:HD1	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:HH12	1:C:251:LYS:HB2	1.87	0.40
1:C:393:GLY:O	1:C:587:THR:HG23	2.21	0.40
1:D:4:PHE:CE2	1:D:20:ILE:HG13	2.57	0.40
1:D:173:GLN:HE21	1:D:173:GLN:HB3	1.56	0.40
1:D:517:ASP:O	1:D:519:ARG:N	2.47	0.40
1:D:621:ASP:OD2	1:D:621:ASP:C	2.63	0.40
1:D:769:LYS:O	1:D:771:PHE:N	2.53	0.40
2:E:7:DA:H1'	2:E:8:DT:C6	2.57	0.40
2:E:7:DA:H1'	2:E:8:DT:H5'	2.04	0.40
2:I:7:DA:C8	2:I:8:DT:H72	2.56	0.40
1:B:52:ILE:O	1:B:428:GLU:HG3	2.22	0.40
1:B:274:ILE:CG2	1:B:275:ASP:N	2.83	0.40
1:B:397:LYS:O	1:B:399:PRO:HD3	2.21	0.40
1:B:425:ILE:O	1:B:472:PRO:HD3	2.22	0.40
1:B:458:PRO:HG3	1:B:592:MET:SD	2.61	0.40
1:C:109:ARG:NH1	1:C:109:ARG:HG3	2.36	0.40
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.57	0.40
1:C:511:ASP:CA	1:C:534:SER:HB2	2.51	0.40
1:C:525:GLU:CD	1:C:525:GLU:N	2.74	0.40
1:C:560:LYS:HG2	1:C:564:ASN:HD21	1.86	0.40
1:C:645:ASN:OD1	1:C:719:ARG:NH1	2.52	0.40
1:D:461:MET:HG2	1:D:463:TYR:OH	2.21	0.40
1:D:771:PHE:CD2	1:D:872:LEU:HD13	2.56	0.40
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.56	0.40
1:A:273:TYR:CE1	1:A:335:ASP:OD2	2.74	0.40
1:A:284:ASN:ND2	1:A:285:GLN:N	2.70	0.40
1:A:376:GLN:HE21	1:A:378:LYS:HE3	1.87	0.40
1:A:765:LYS:HB2	1:A:765:LYS:HE3	1.91	0.40
1:A:825:VAL:HG22	1:A:828:GLU:CG	2.45	0.40
1:B:471:VAL:O	1:B:475:ILE:HG22	2.22	0.40
1:B:738:PRO:O	1:B:739:LYS:C	2.65	0.40
1:C:161:GLU:H	1:C:161:GLU:HG2	1.70	0.40
1:C:507:ASN:HD22	1:C:508:LEU:H	1.63	0.40
1:D:75:MET:HE3	1:D:75:MET:HB3	1.98	0.40
1:D:176:ASP:OD1	1:D:318:GLN:HG3	2.21	0.40
1:D:283:THR:OG1	1:D:285:GLN:NE2	2.55	0.40
1:D:741:VAL:C	1:D:743:LYS:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	900/906 (99%)	824 (92%)	71 (8%)	5 (1%)	21	53
1	B	900/906 (99%)	822 (91%)	68 (8%)	10 (1%)	11	40
1	C	899/906 (99%)	803 (89%)	83 (9%)	13 (1%)	9	34
1	D	895/906 (99%)	764 (85%)	103 (12%)	28 (3%)	3	16
All	All	3594/3624 (99%)	3213 (89%)	325 (9%)	56 (2%)	7	31

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	A	515	ASP
1	B	300	VAL
1	B	518	TYR
1	C	45	GLN
1	C	300	VAL
1	C	534	SER
1	D	161	GLU
1	D	315	SER
1	D	622	THR
1	D	732	THR
1	D	757	GLU
1	D	895	ALA
1	A	45	GLN
1	B	45	GLN
1	B	304	LYS
1	B	898	PHE
1	C	304	LYS
1	C	458	PRO
1	C	492	ALA
1	C	509	SER
1	C	510	VAL

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Mol	Chain	Res	Type
1	C	896	SER
1	D	45	GLN
1	D	136	ILE
1	D	181	GLU
1	D	508	LEU
1	D	733	GLN
1	D	819	ILE
1	D	859	LYS
1	A	900	MET
1	B	524	ASP
1	B	525	GLU
1	C	415	LEU
1	C	494	ARG
1	D	199	MET
1	D	522	PHE
1	D	822	PRO
1	A	519	ARG
1	B	414	SER
1	C	522	PHE
1	D	179	PRO
1	D	414	SER
1	D	458	PRO
1	D	518	TYR
1	D	734	LYS
1	D	770	GLU
1	D	771	PHE
1	B	458	PRO
1	D	388	VAL
1	D	524	ASP
1	B	561	LEU
1	D	222	ALA
1	D	244	PRO
1	C	505	ASN
1	D	187	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	781/803 (97%)	724 (93%)	57 (7%)	13	40
1	B	788/803 (98%)	738 (94%)	50 (6%)	16	46
1	C	788/803 (98%)	732 (93%)	56 (7%)	13	41
1	D	758/803 (94%)	682 (90%)	76 (10%)	7	27
All	All	3115/3212 (97%)	2876 (92%)	239 (8%)	12	38

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	45	GLN
1	A	47	THR
1	A	48	LYS
1	A	64	ASN
1	A	70	GLN
1	A	105	HIS
1	A	106	THR
1	A	193	ASN
1	A	199	MET
1	A	207	GLN
1	A	213	LEU
1	A	218	VAL
1	A	219	GLU
1	A	220	SER
1	A	229	ARG
1	A	231	LYS
1	A	242	LEU
1	A	246	ARG
1	A	251	LYS
1	A	260	ARG
1	A	261	GLU
1	A	276	LEU
1	A	283	THR
1	A	311	LYS
1	A	318	GLN
1	A	332	LEU
1	A	358	VAL
1	A	362	ILE
1	A	372	SER
1	A	379	VAL
1	A	384	ARG
1	A	414	SER

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Mol	Chain	Res	Type
1	A	446	VAL
1	A	468	ASP
1	A	477	LYS
1	A	483	LYS
1	A	505	ASN
1	A	543	PHE
1	A	592	MET
1	A	612	GLU
1	A	614	GLU
1	A	645	ASN
1	A	658	ARG
1	A	685	ARG
1	A	703	THR
1	A	706	LYS
1	A	728	MET
1	A	731	GLU
1	A	734	LYS
1	A	745	LEU
1	A	777	ILE
1	A	790	LYS
1	A	825	VAL
1	A	829	LYS
1	A	861	ASP
1	A	863	LEU
1	B	9	GLU
1	B	34	LYS
1	B	45	GLN
1	B	47	THR
1	B	93	LEU
1	B	112	ASN
1	B	114	ASP
1	B	116	GLU
1	B	128	GLN
1	B	148	VAL
1	B	154	SER
1	B	164	ILE
1	B	173	GLN
1	B	185	LYS
1	B	193	ASN
1	B	253	ILE
1	B	257	TYR
1	B	302	LYS

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Mol	Chain	Res	Type
1	B	319	ARG
1	B	341	ILE
1	B	363	LYS
1	B	372	SER
1	B	421	ARG
1	B	479	PHE
1	B	503	LEU
1	B	531	LYS
1	B	532	LYS
1	B	533	LEU
1	B	538	LEU
1	B	542	LEU
1	B	544	ARG
1	B	549	GLU
1	B	558	ASN
1	B	573	VAL
1	B	597	ILE
1	B	618	LEU
1	B	631	LYS
1	B	632	ILE
1	B	639	SER
1	B	649	ASP
1	B	658	ARG
1	B	660	GLU
1	B	672	GLU
1	B	685	ARG
1	B	728	MET
1	B	773	GLN
1	B	819	ILE
1	B	820	ASP
1	B	843	ASP
1	B	885	SER
1	C	18	ARG
1	C	26	GLU
1	C	38	PHE
1	C	43	GLU
1	C	58	THR
1	C	64	ASN
1	C	65	MET
1	C	73	LYS
1	C	83	LEU
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	93	LEU
1	C	127	SER
1	C	149	PHE
1	C	161	GLU
1	C	206	GLN
1	C	217	ASN
1	C	238	THR
1	C	302	LYS
1	C	313	ARG
1	C	314	GLU
1	C	326	ILE
1	C	356	GLN
1	C	375	GLU
1	C	408	MET
1	C	414	SER
1	C	426	SER
1	C	428	GLU
1	C	429	THR
1	C	440	HIS
1	C	456	CYS
1	C	461	MET
1	C	466	ASP
1	C	467	ARG
1	C	474	GLU
1	C	479	PHE
1	C	494	ARG
1	C	517	ASP
1	C	525	GLU
1	C	533	LEU
1	C	556	GLN
1	C	562	LEU
1	C	572	ASN
1	C	587	THR
1	C	599	ARG
1	C	614	GLU
1	C	686	GLU
1	C	746	LYS
1	C	752	MET
1	C	760	LEU
1	C	781	SER
1	C	806	ARG
1	C	819	ILE

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Mol	Chain	Res	Type
1	C	843	ASP
1	C	880	LEU
1	C	898	PHE
1	C	900	MET
1	D	2	LYS
1	D	8	VAL
1	D	10	GLN
1	D	31	VAL
1	D	32	GLU
1	D	36	SER
1	D	45	GLN
1	D	61	LEU
1	D	93	LEU
1	D	104	ASP
1	D	105	HIS
1	D	133	ILE
1	D	136	ILE
1	D	147	TYR
1	D	151	LEU
1	D	164	ILE
1	D	165	GLU
1	D	173	GLN
1	D	181	GLU
1	D	194	GLU
1	D	213	LEU
1	D	250	VAL
1	D	264	THR
1	D	270	VAL
1	D	285	GLN
1	D	290	LEU
1	D	297	GLU
1	D	303	LEU
1	D	305	TYR
1	D	361	PRO
1	D	362	ILE
1	D	363	LYS
1	D	391	TYR
1	D	395	PHE
1	D	401	PRO
1	D	403	ARG
1	D	408	MET
1	D	441	ASP

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Mol	Chain	Res	Type
1	D	452	ASP
1	D	467	ARG
1	D	474	GLU
1	D	479	PHE
1	D	490	LEU
1	D	494	ARG
1	D	521	ASP
1	D	525	GLU
1	D	536	LYS
1	D	557	ILE
1	D	558	ASN
1	D	562	LEU
1	D	581	ARG
1	D	594	LEU
1	D	599	ARG
1	D	612	GLU
1	D	614	GLU
1	D	618	LEU
1	D	621	ASP
1	D	630	ASP
1	D	646	HIS
1	D	658	ARG
1	D	660	GLU
1	D	667	PHE
1	D	684	ASP
1	D	706	LYS
1	D	710	LEU
1	D	725	LEU
1	D	739	LYS
1	D	766	GLU
1	D	777	ILE
1	D	826	GLU
1	D	830	VAL
1	D	848	TRP
1	D	873	GLU
1	D	881	GLU
1	D	883	PHE
1	D	894	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	40	HIS
1	A	64	ASN
1	A	98	ASN
1	A	112	ASN
1	A	138	HIS
1	A	153	ASN
1	A	158	ASN
1	A	171	GLN
1	A	173	GLN
1	A	193	ASN
1	A	206	GLN
1	A	207	GLN
1	A	217	ASN
1	A	284	ASN
1	A	285	GLN
1	A	333	GLN
1	A	376	GLN
1	A	386	HIS
1	A	389	GLN
1	A	422	GLN
1	A	505	ASN
1	A	556	GLN
1	A	558	ASN
1	A	572	ASN
1	A	602	ASN
1	A	645	ASN
1	A	646	HIS
1	A	678	GLN
1	A	711	ASN
1	A	733	GLN
1	A	786	ASN
1	A	839	ASN
1	A	864	HIS
1	B	105	HIS
1	B	171	GLN
1	B	173	GLN
1	B	316	ASN
1	B	318	GLN
1	B	324	ASN
1	B	354	GLN
1	B	371	ASN
1	B	376	GLN

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Mol	Chain	Res	Type
1	B	505	ASN
1	B	507	ASN
1	B	539	ASN
1	B	558	ASN
1	B	595	GLN
1	B	645	ASN
1	B	733	GLN
1	B	754	GLN
1	B	823	GLN
1	C	10	GLN
1	C	40	HIS
1	C	131	HIS
1	C	203	ASN
1	C	206	GLN
1	C	207	GLN
1	C	232	ASN
1	C	255	ASN
1	C	284	ASN
1	C	285	GLN
1	C	299	ASN
1	C	318	GLN
1	C	324	ASN
1	C	377	ASN
1	C	402	ASN
1	C	424	ASN
1	C	444	ASN
1	C	493	GLN
1	C	507	ASN
1	C	546	GLN
1	C	556	GLN
1	C	558	ASN
1	C	564	ASN
1	C	572	ASN
1	C	582	ASN
1	C	595	GLN
1	C	675	ASN
1	C	676	ASN
1	C	678	GLN
1	C	679	HIS
1	C	711	ASN
1	C	733	GLN
1	C	775	ASN

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Mol	Chain	Res	Type
1	C	786	ASN
1	C	787	ASN
1	C	818	ASN
1	C	823	GLN
1	D	64	ASN
1	D	105	HIS
1	D	112	ASN
1	D	153	ASN
1	D	158	ASN
1	D	206	GLN
1	D	285	GLN
1	D	333	GLN
1	D	354	GLN
1	D	377	ASN
1	D	382	GLN
1	D	424	ASN
1	D	444	ASN
1	D	480	ASN
1	D	505	ASN
1	D	546	GLN
1	D	556	GLN
1	D	558	ASN
1	D	595	GLN
1	D	602	ASN
1	D	606	ASN
1	D	675	ASN
1	D	678	GLN
1	D	742	GLN
1	D	754	GLN
1	D	761	GLN
1	D	773	GLN
1	D	775	ASN
1	D	812	ASN
1	D	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	I	4	2,3	18,23,24	0.89	1 (5%)	21,35,38	0.73	1 (4%)
2	CTG	G	4	2,3	18,23,24	0.79	0	21,35,38	0.86	1 (4%)
2	CTG	K	4	2	18,23,24	0.84	1 (5%)	21,35,38	0.66	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C1'-N1	2.87	1.49	1.45
2	K	4	CTG	C1'-N1	2.36	1.48	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	CTG	N3-C2-N1	-2.64	114.02	116.78
2	G	4	CTG	N3-C2-N1	-2.18	114.50	116.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DTP	B	907	-	31,32,32	0.56	0	46,50,50	0.74	1 (2%)
4	DTP	J	2	-	31,32,32	0.56	0	46,50,50	0.64	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	B	907	-	-	7/22/34/34	0/3/3/3
4	DTP	J	2	-	-	5/22/34/34	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	DTP	O2G-PG-O1G	2.19	119.38	110.83
4	J	2	DTP	O2G-PG-O1G	2.15	119.22	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

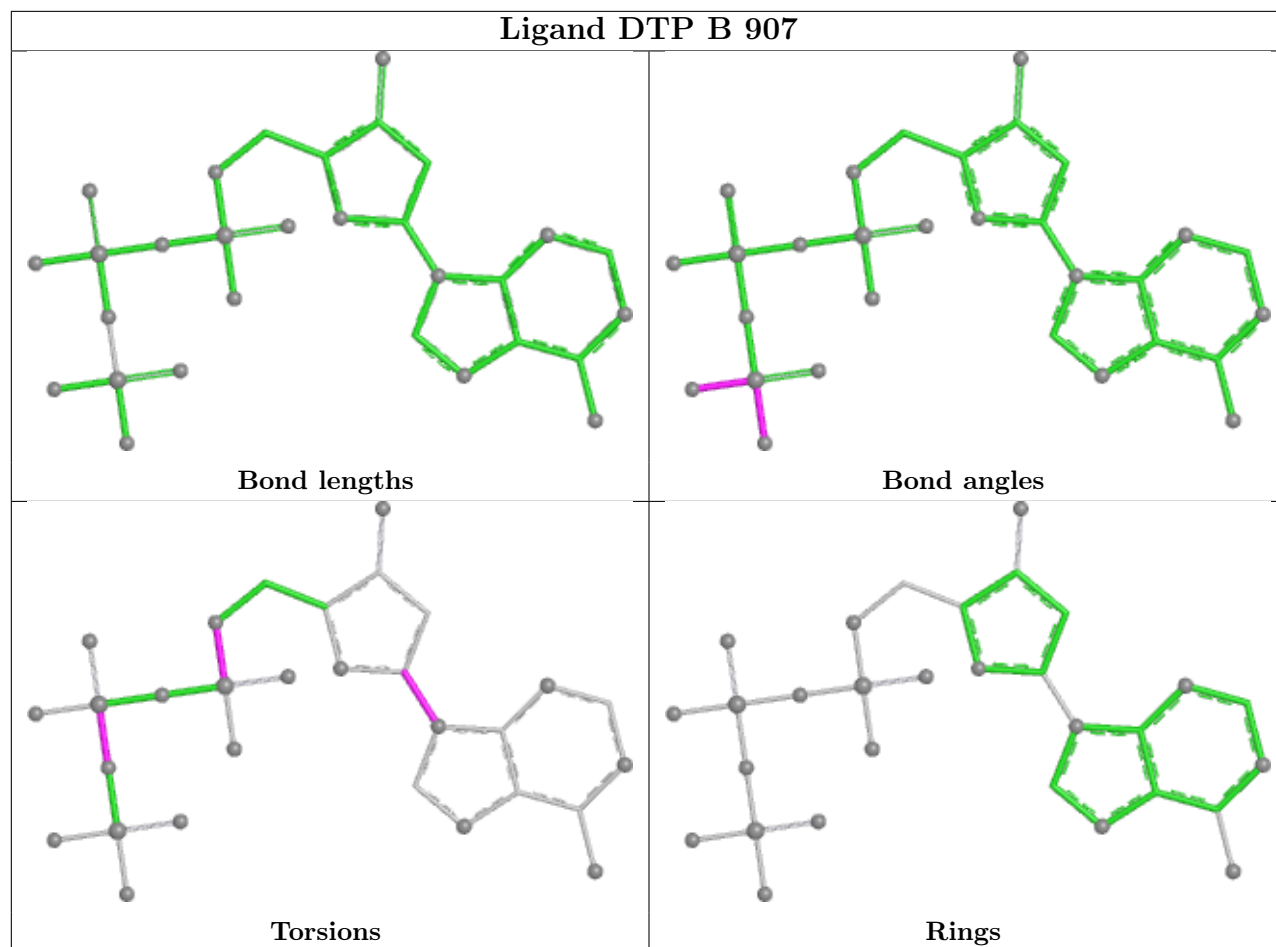
Mol	Chain	Res	Type	Atoms
4	B	907	DTP	C5'-O5'-PA-O2A
4	B	907	DTP	C5'-O5'-PA-O3A
4	B	907	DTP	O4'-C1'-N9-C4
4	J	2	DTP	C5'-O5'-PA-O3A
4	B	907	DTP	O4'-C1'-N9-C8
4	J	2	DTP	O4'-C1'-N9-C8
4	B	907	DTP	PG-O3B-PB-O1B
4	B	907	DTP	C5'-O5'-PA-O1A
4	J	2	DTP	C5'-O5'-PA-O1A
4	B	907	DTP	PG-O3B-PB-O2B
4	J	2	DTP	O4'-C1'-N9-C4
4	J	2	DTP	PA-O3A-PB-O2B

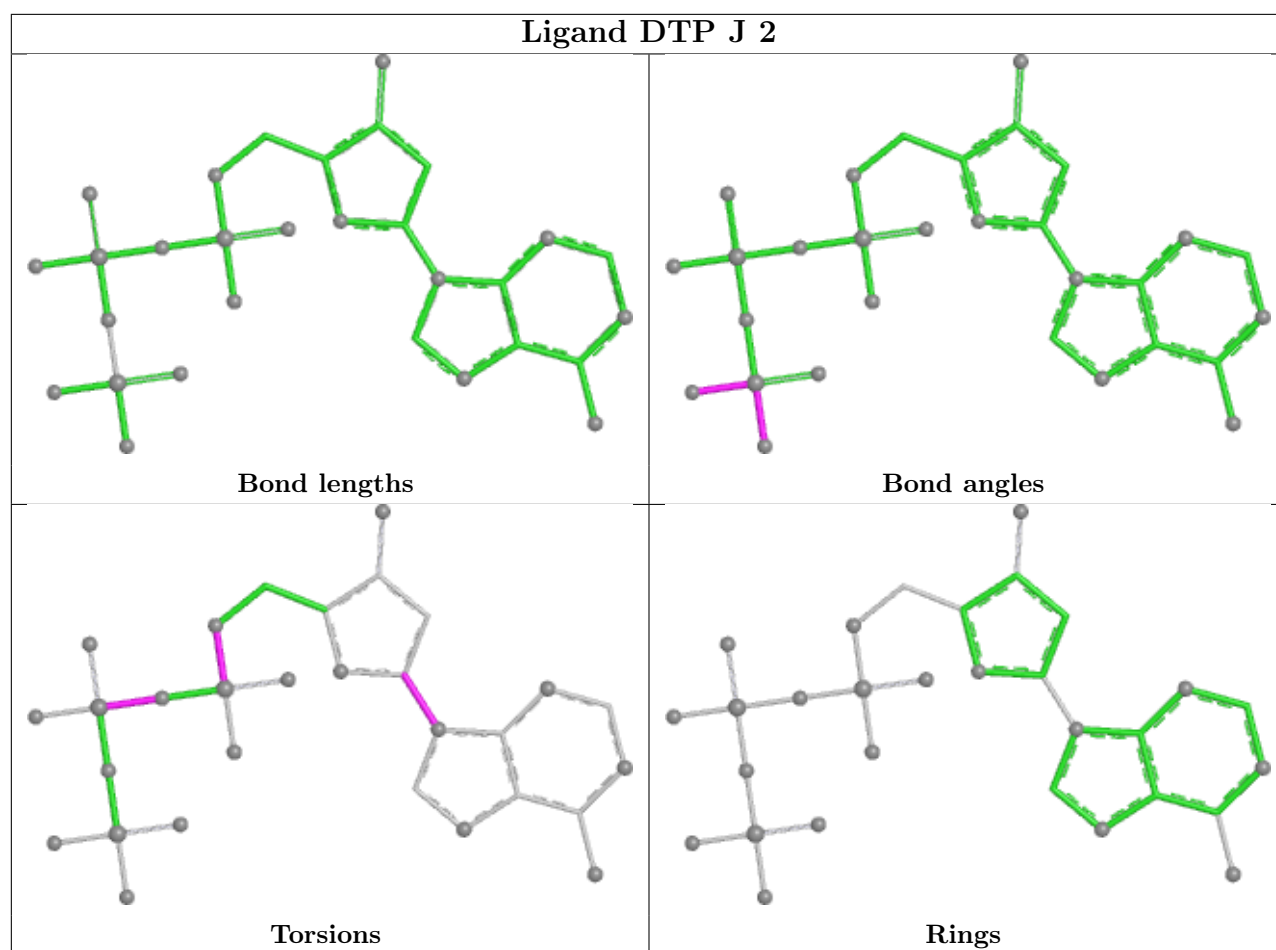
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	907	DTP	3	0
4	J	2	DTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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%)	0.22	36 (3%)	42	26	23, 52, 158, 200	0
1	B	902/906 (99%)	0.19	27 (2%)	52	34	27, 53, 146, 170	0
1	C	901/906 (99%)	0.34	48 (5%)	32	19	21, 55, 145, 173	0
1	D	897/906 (99%)	0.60	60 (6%)	24	14	37, 70, 126, 170	1 (0%)
2	E	13/18 (72%)	1.10	1 (7%)	19	12	69, 110, 130, 135	0
2	G	17/18 (94%)	0.12	0	100	100	52, 72, 106, 106	0
2	I	17/18 (94%)	-0.10	0	100	100	36, 53, 88, 96	0
2	K	17/18 (94%)	0.79	0	100	100	39, 105, 142, 145	0
3	F	13/15 (86%)	1.43	2 (15%)	5	3	94, 121, 139, 140	0
3	H	15/15 (100%)	0.39	1 (6%)	24	14	45, 79, 149, 150	0
3	J	15/15 (100%)	-0.10	0	100	100	36, 63, 121, 124	0
3	L	15/15 (100%)	0.77	0	100	100	82, 116, 141, 145	0
All	All	3724/3756 (99%)	0.34	175 (4%)	36	22	21, 57, 140, 200	1 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	394	ALA	6.3
1	D	393	GLY	5.9
1	D	825	VAL	5.7
1	A	510	VAL	5.6
1	D	395	PHE	5.6
1	C	535	ALA	5.6
1	C	303	LEU	5.4
1	D	391	TYR	5.3
1	C	514	LEU	5.1
1	C	510	VAL	5.0
1	D	498	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	514	LEU	4.6
1	C	526	ILE	4.5
1	D	510	VAL	4.4
1	D	390	PRO	4.4
1	D	392	PRO	4.4
1	A	508	LEU	4.3
1	C	253	ILE	4.3
1	C	499	ILE	4.2
1	B	499	ILE	4.1
1	C	252	VAL	4.1
1	C	533	LEU	3.9
1	C	498	ILE	3.8
1	D	396	VAL	3.8
1	C	530	ILE	3.8
1	A	498	ILE	3.8
1	C	257	TYR	3.8
1	B	545	ALA	3.7
1	D	520	PHE	3.6
1	A	518	TYR	3.6
1	C	522	PHE	3.6
1	A	530	ILE	3.6
1	B	253	ILE	3.6
1	D	518	TYR	3.6
1	C	503	LEU	3.6
1	D	625	ILE	3.5
1	D	389	GLN	3.4
1	D	252	VAL	3.4
1	C	513	PRO	3.4
1	A	542	LEU	3.3
1	C	901	PHE	3.3
1	C	256	MET	3.3
1	B	252	VAL	3.3
1	A	785	ALA	3.2
1	C	504	HIS	3.2
1	B	530	ILE	3.2
1	C	516	VAL	3.2
1	D	157	GLY	3.2
1	A	543	PHE	3.1
1	A	526	ILE	3.1
1	D	253	ILE	3.1
1	D	410	PHE	3.1
1	C	536	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	526	ILE	3.1
1	C	518	TYR	3.0
1	C	496	GLY	3.0
3	F	101	DG	3.0
1	B	522	PHE	3.0
1	B	550	VAL	3.0
1	C	500	LYS	3.0
1	A	535	ALA	3.0
1	C	505	ASN	3.0
1	A	548	THR	2.9
1	D	516	VAL	2.9
1	D	526	ILE	2.9
1	A	516	VAL	2.9
1	D	522	PHE	2.9
1	A	252	VAL	2.9
1	A	728	MET	2.9
1	A	303	LEU	2.9
1	B	303	LEU	2.9
1	D	314	GLU	2.8
3	H	101	DG	2.8
1	A	509	SER	2.8
1	A	520	PHE	2.8
1	B	498	ILE	2.8
1	A	539	ASN	2.8
1	D	824	VAL	2.7
1	B	502	ALA	2.7
1	D	304	LYS	2.7
1	B	508	LEU	2.7
1	A	541	MET	2.6
1	A	257	TYR	2.6
1	D	279	LYS	2.6
1	D	508	LEU	2.6
1	B	256	MET	2.6
1	D	155	PRO	2.6
1	C	528	GLU	2.6
1	A	536	LYS	2.6
1	D	250	VAL	2.6
1	C	531	LYS	2.5
1	D	305	TYR	2.5
1	C	78	ILE	2.5
1	B	528	GLU	2.5
1	B	520	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	309	ILE	2.5
1	D	636	VAL	2.5
3	F	113	DC	2.5
1	D	897	LEU	2.5
1	A	784	SER	2.5
1	B	531	LYS	2.5
1	C	529	LYS	2.5
1	A	537	SER	2.4
1	D	178	VAL	2.4
1	C	520	PHE	2.4
1	C	495	ASN	2.4
1	A	819	ILE	2.4
1	D	164	ILE	2.4
1	A	828	GLU	2.4
1	C	508	LEU	2.4
1	C	541	MET	2.4
1	C	155	PRO	2.4
1	D	827	GLY	2.4
1	C	525	GLU	2.4
1	D	512	GLU	2.4
1	B	897	LEU	2.4
1	C	539	ASN	2.4
1	D	622	THR	2.4
1	A	301	GLY	2.3
1	B	496	GLY	2.3
1	D	156	TYR	2.3
1	C	519	ARG	2.3
1	D	303	LEU	2.3
1	D	527	LYS	2.3
1	A	612	GLU	2.3
1	B	114	ASP	2.3
1	D	521	ASP	2.3
1	D	312	LEU	2.3
1	D	726	LYS	2.3
1	B	255	ASN	2.3
1	A	254	GLU	2.3
1	C	527	LYS	2.3
1	D	729	GLY	2.3
1	D	282	PHE	2.2
1	D	187	ILE	2.2
1	A	504	HIS	2.2
1	D	848	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	509	SER	2.2
1	C	174	GLY	2.2
1	C	487	GLY	2.2
1	C	502	ALA	2.2
1	D	172	GLU	2.2
2	E	6	DA	2.2
1	C	194	GLU	2.2
1	D	530	ILE	2.2
1	B	257	TYR	2.2
1	B	503	LEU	2.2
1	D	398	GLU	2.2
1	D	623	ASP	2.2
1	C	545	ALA	2.2
1	D	728	MET	2.1
1	A	897	LEU	2.1
1	C	542	LEU	2.1
1	B	510	VAL	2.1
1	D	251	LYS	2.1
1	D	170	LEU	2.1
1	D	513	PRO	2.1
1	D	692	PRO	2.1
1	B	79	GLY	2.1
1	B	514	LEU	2.1
1	C	301	GLY	2.1
1	D	115	ILE	2.1
1	A	506	PRO	2.1
1	A	502	ALA	2.1
1	B	529	LYS	2.0
1	D	523	SER	2.0
1	C	538	LEU	2.0
1	B	548	THR	2.0
1	A	515	ASP	2.0
1	A	521	ASP	2.0
1	C	515	ASP	2.0
1	D	531	LYS	2.0
1	A	256	MET	2.0
1	C	323	TYR	2.0
1	A	793	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CTG	K	4	22/23	0.72	0.15	134,145,148,148	0
2	CTG	I	4	22/23	0.81	0.14	79,88,93,95	0
2	CTG	G	4	22/23	0.91	0.10	71,76,79,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

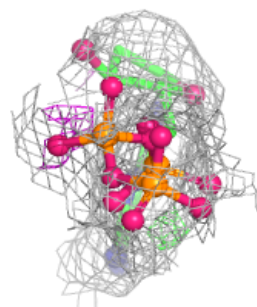
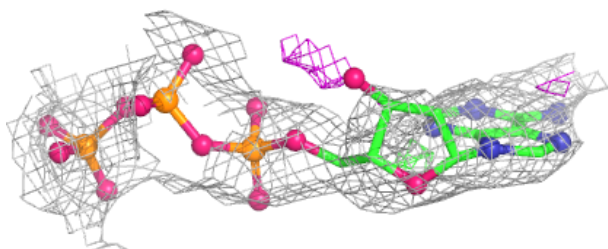
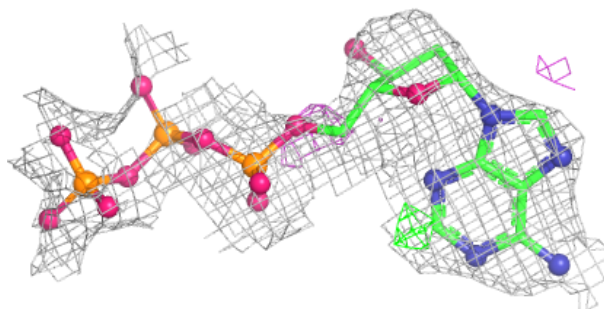
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DTP	J	2	30/30	0.77	0.17	140,147,166,166	0
4	DTP	B	907	30/30	0.78	0.17	133,137,151,151	0

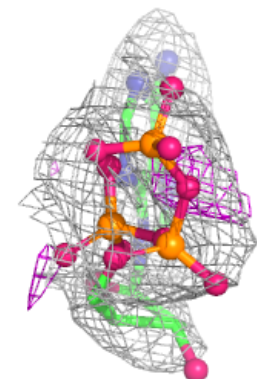
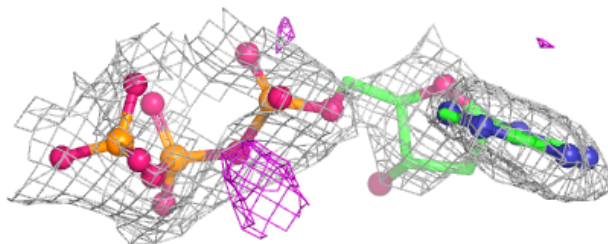
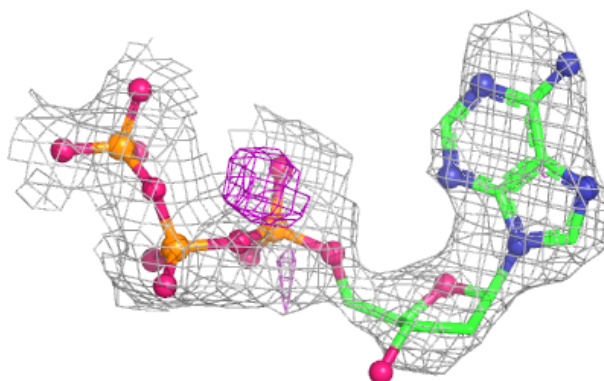
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DTP J 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DTP B 907:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.