



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:15 AM UTC

PDB ID : 3RMC / pdb_00003rmc
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 : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
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

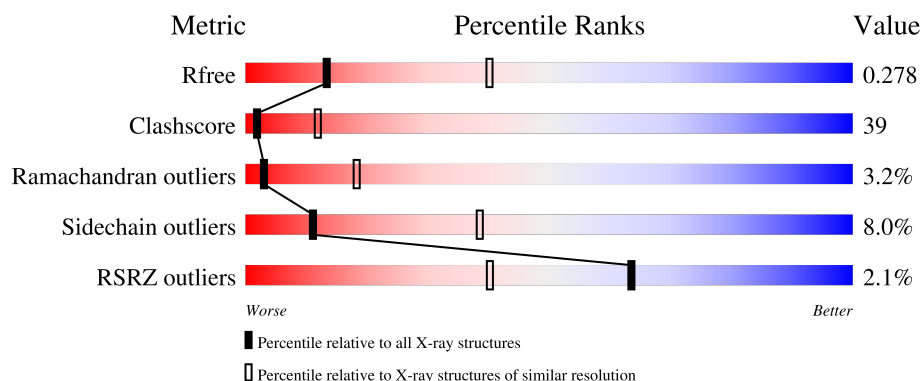
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



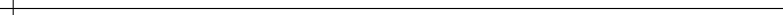
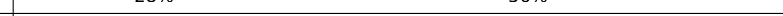
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	41% 49% 9%
1	B	906	2% 43% 49% 7%
1	C	906	45% 48% 6%
1	D	906	4% 34% 56% 9%
2	E	18	33% 61% 6%

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Mol	Chain	Length	Quality of chain
2	G	18	
2	I	18	
2	K	18	
3	F	14	
3	H	14	
3	J	14	
3	L	14	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31561 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			7323	4704	1220	1367	32			
1	B	902	Total	C	N	O	S	13	0	0
			7246	4643	1202	1368	33			
1	C	901	Total	C	N	O	S	0	0	0
			7339	4712	1220	1374	33			
1	D	890	Total	C	N	O	S	15	0	0
			7027	4507	1155	1334	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
C	904	HIS	-	expression tag	UNP Q38087
C	905	HIS	-	expression tag	UNP Q38087
C	906	HIS	-	expression tag	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087
D	904	HIS	-	expression tag	UNP Q38087
D	905	HIS	-	expression tag	UNP Q38087
D	906	HIS	-	expression tag	UNP Q38087

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	33	Total	O	0	0
			33	33		
4	C	32	Total	O	0	0
			32	32		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	G	3	Total	O	0	0
			3	3		
4	H	3	Total	O	0	0
			3	3		
4	I	3	Total	O	0	0
			3	3		

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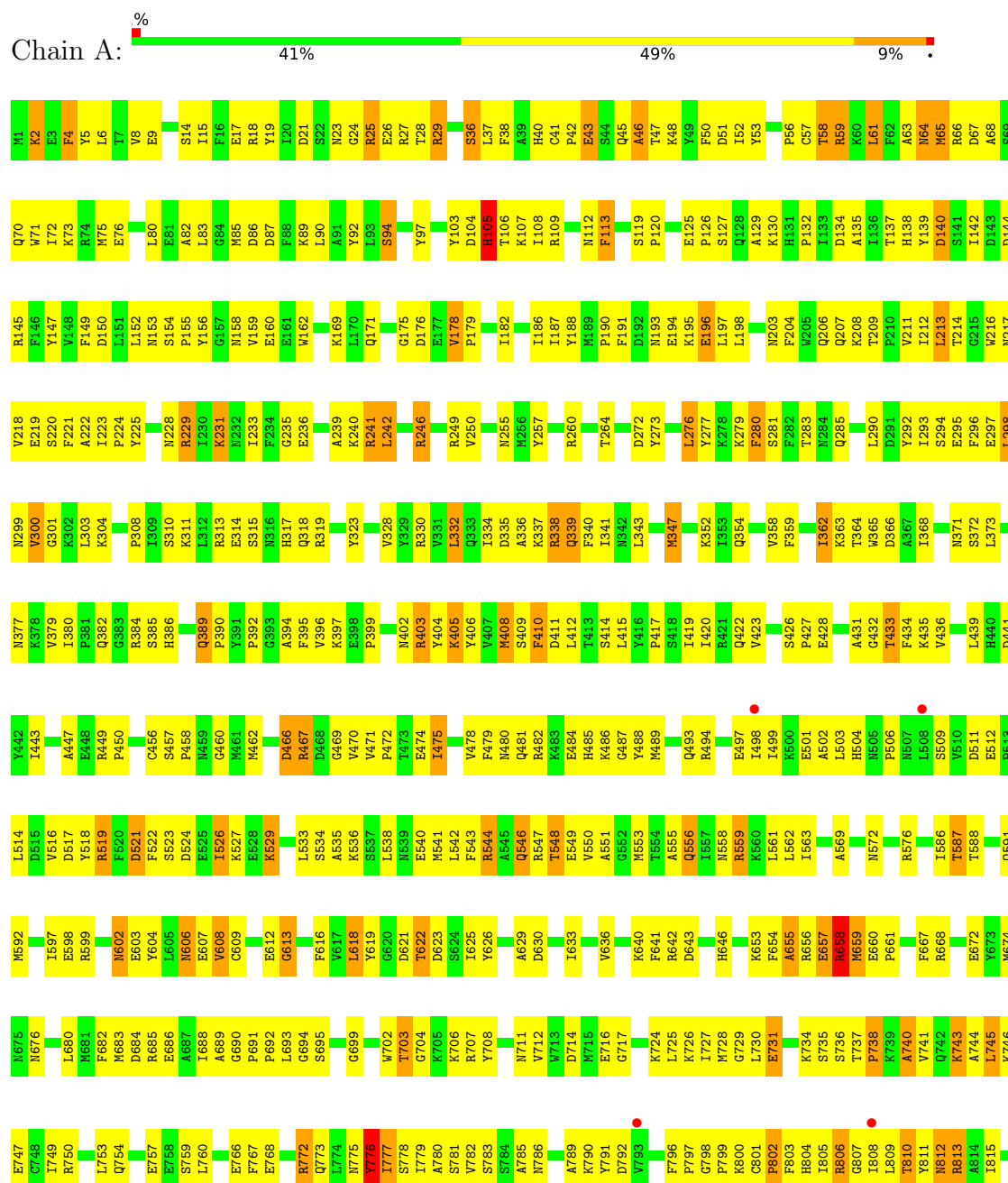
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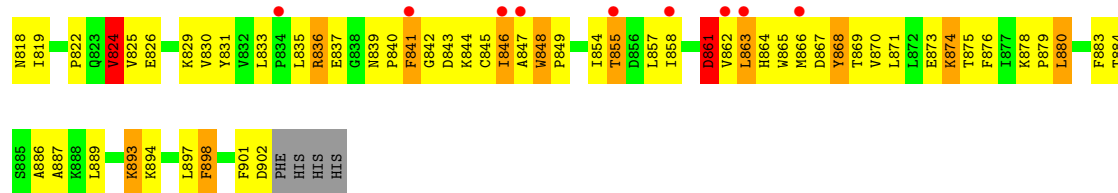
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	O	0	0
			1	1		

3 Residue-property plots

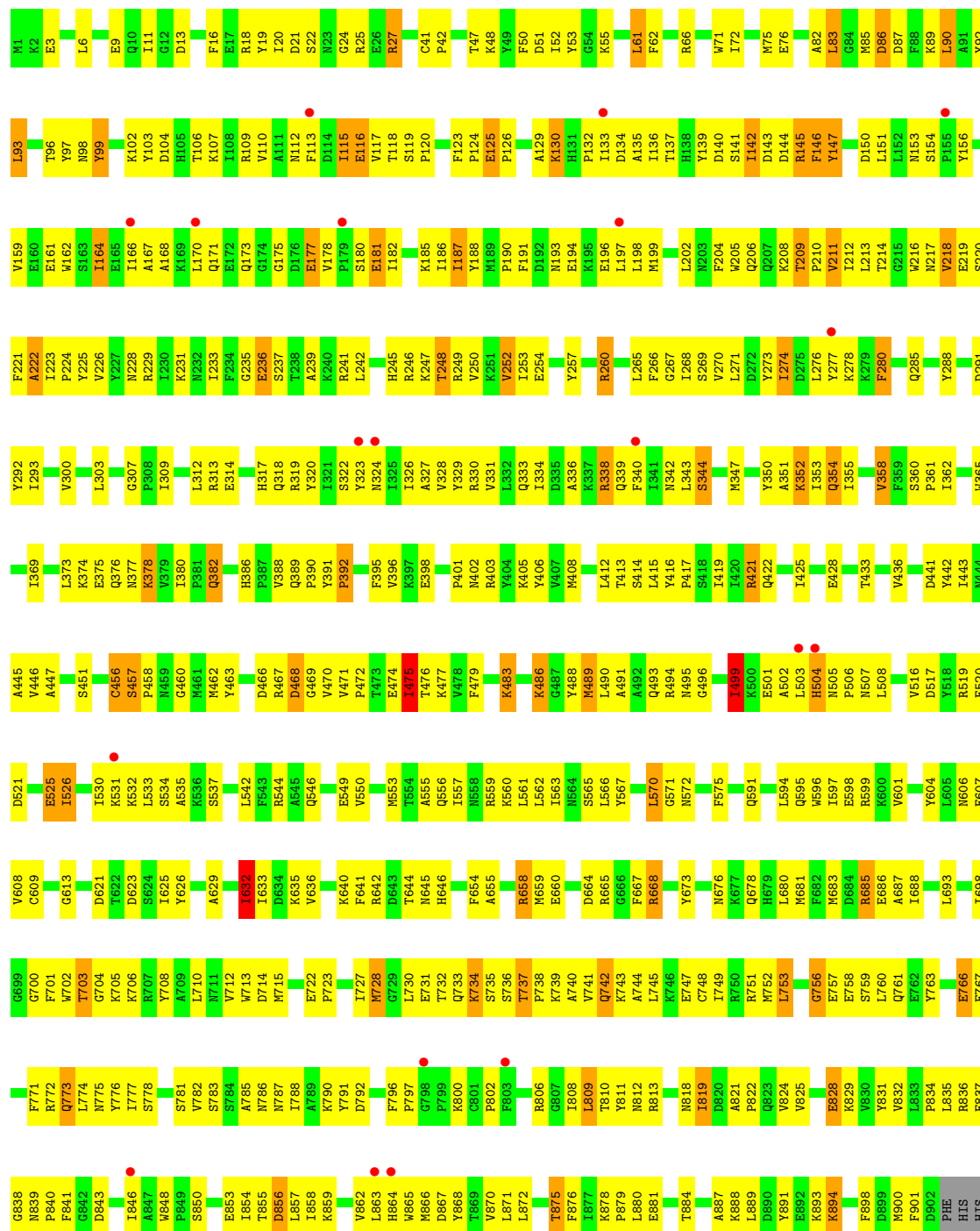
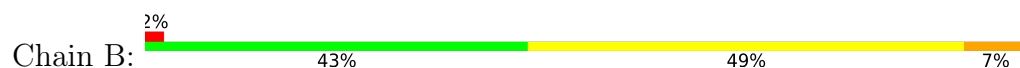
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



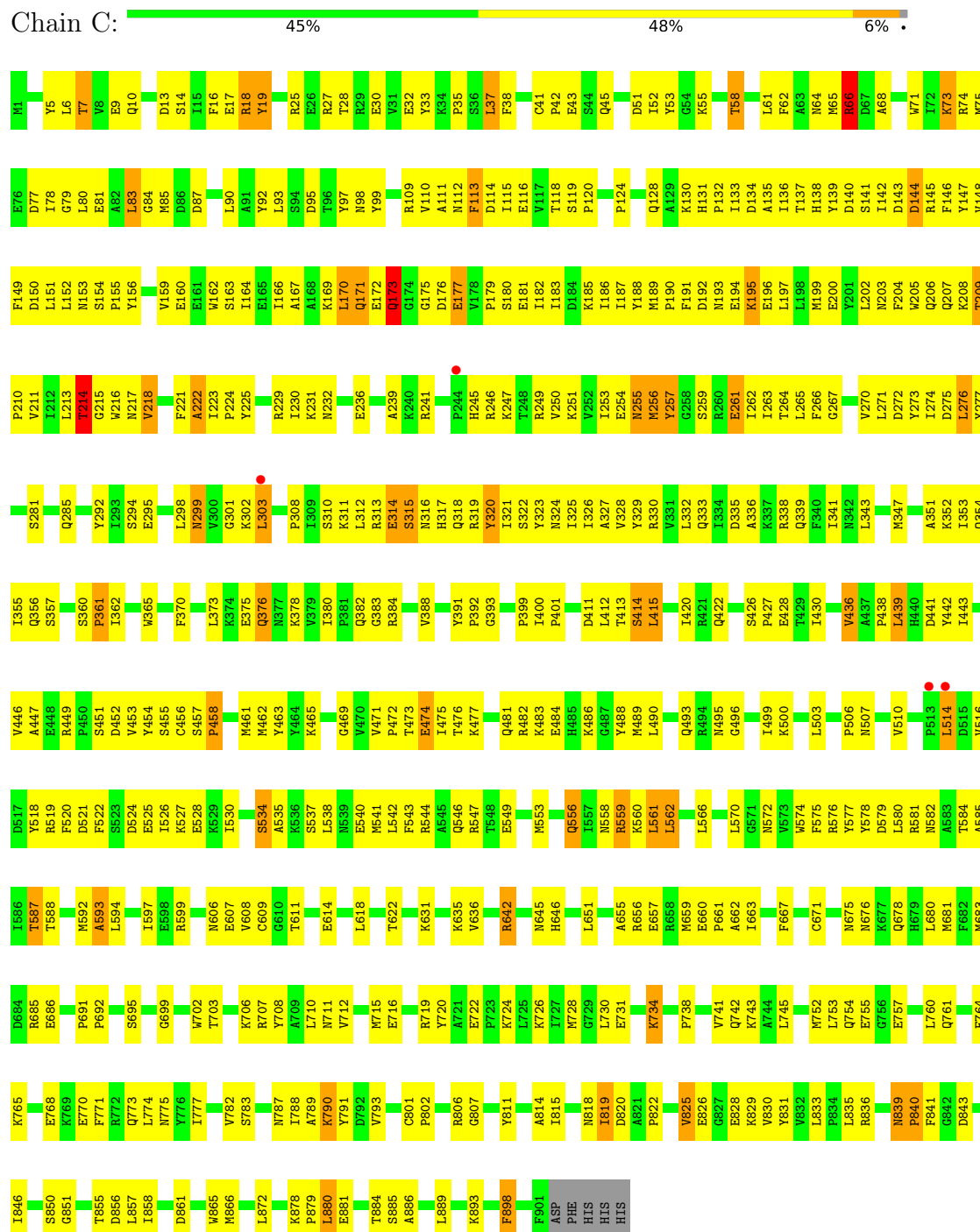


● Molecule 1: DNA polymerase



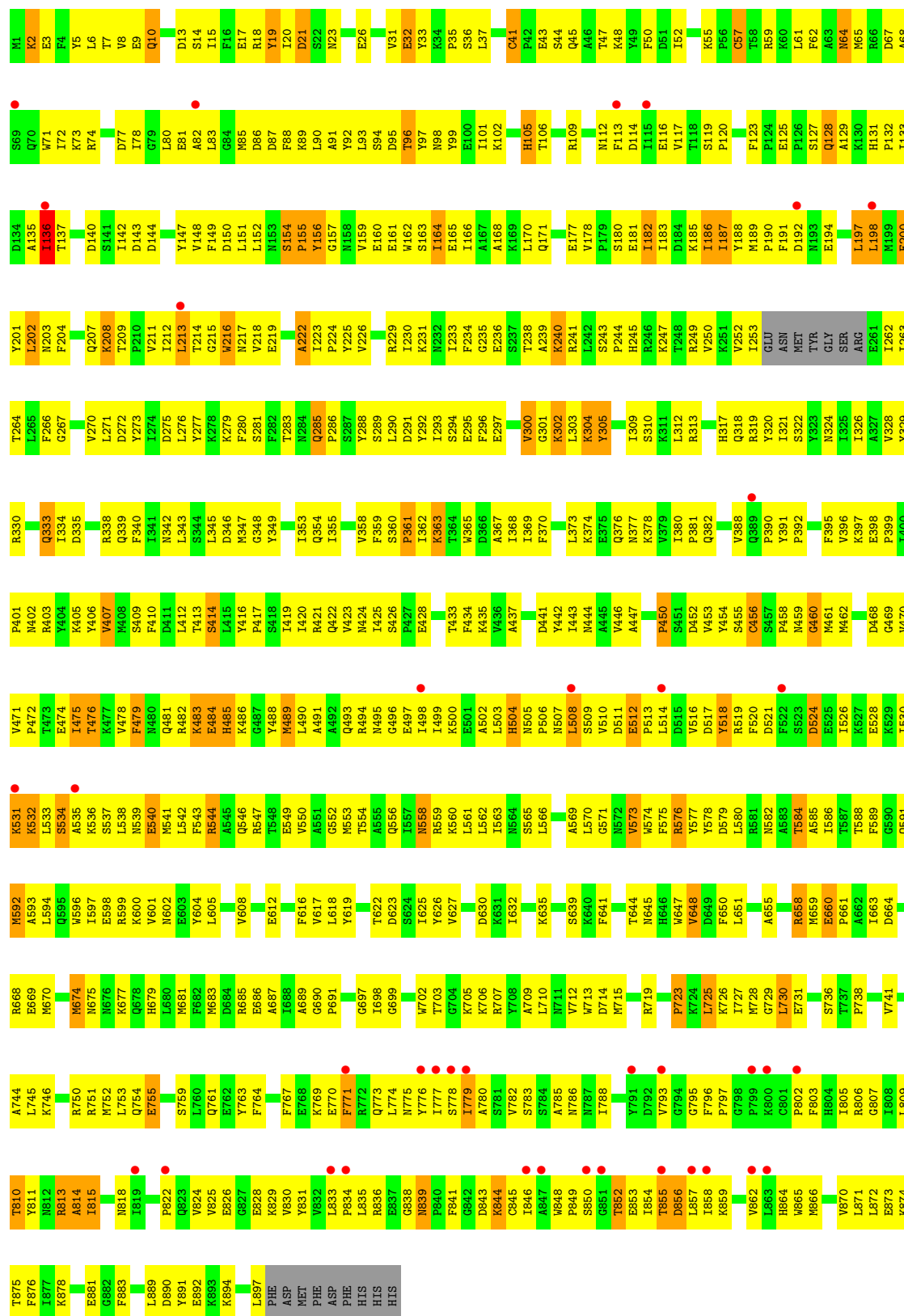
HIS

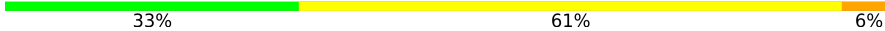
• Molecule 1: DNA polymerase

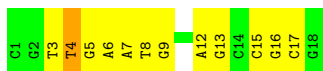


• Molecule 1: DNA polymerase

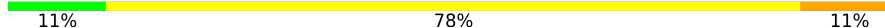


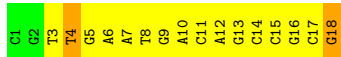


Chain E:  33% 61% 6%



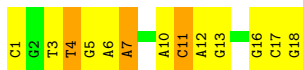
- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain G:  11% 78% 11%



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

Chain I:  28% 56% 17%

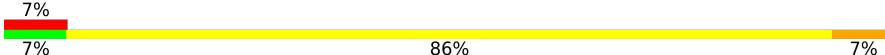


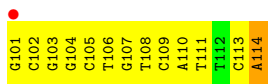
- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain K:  11% 44% 33% 22%

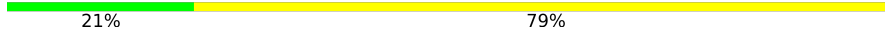


- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain F:  7% 7% 86% 7%



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

Chain H:  21% 79%

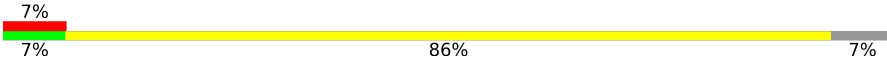


- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain J:  50% 50%



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

Chain L:  7% 7% 86%



G101	C102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	DA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.99Å 123.77Å 163.64Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-3.00) 92.4 (50.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.282 0.217 , 0.278	Depositor DCC
R_{free} test set	19675 reflections (9.40%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31561	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

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

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

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	0.55	0/7503	1.08	47/10148 (0.5%)
1	B	0.50	0/7421	1.00	38/10054 (0.4%)
1	C	0.56	0/7519	1.03	31/10166 (0.3%)
1	D	0.43	0/7198	0.96	31/9779 (0.3%)
2	E	0.33	0/390	0.70	0/598
2	G	0.30	0/390	0.63	1/598 (0.2%)
2	I	0.43	0/390	0.82	2/598 (0.3%)
2	K	0.28	0/323	0.55	0/497
3	F	0.30	0/315	0.74	0/484
3	H	0.29	0/315	0.64	0/484
3	J	0.42	0/315	0.90	0/484
3	L	0.27	0/292	0.59	0/449
All	All	0.50	0/32371	0.99	150/44339 (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
1	A	0	1
2	I	0	2
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	THR	N-CA-C	-10.68	100.36	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	VAL	N-CA-C	-10.64	102.78	113.10
1	D	165	GLU	N-CA-C	-9.70	100.71	111.28
1	D	475	ILE	N-CA-C	-9.68	103.99	112.12
1	D	838	GLY	N-CA-C	-9.50	101.87	115.27
1	A	178	VAL	N-CA-C	-9.31	99.83	108.95
1	A	338	ARG	N-CA-C	8.67	123.61	112.34
1	A	178	VAL	CA-C-N	8.62	129.15	119.93
1	A	178	VAL	C-N-CA	8.62	129.15	119.93
1	B	338	ARG	N-CA-C	8.46	120.27	111.14
1	A	456	CYS	N-CA-C	8.08	121.75	109.23
1	D	540	GLU	N-CA-C	-8.03	103.62	113.50
1	B	598	GLU	N-CA-C	-7.76	101.80	111.11
1	B	839	ASN	CA-C-N	7.64	127.36	119.56
1	B	839	ASN	C-N-CA	7.64	127.36	119.56
1	D	489	MET	N-CA-C	-7.63	104.10	113.41
1	D	476	THR	N-CA-C	-7.63	103.85	113.01
1	B	756	GLY	N-CA-C	7.58	119.88	111.85
1	D	361	PRO	N-CA-C	-7.50	104.81	114.03
1	A	519	ARG	N-CA-C	-7.38	103.26	111.82
1	D	755	GLU	N-CA-C	7.36	118.99	110.97
1	D	154	SER	N-CA-C	7.26	114.75	108.22
1	B	161	GLU	N-CA-C	7.11	119.40	109.31
2	I	18	DG	C2'-C3'-O3'	-6.99	101.02	111.50
1	A	18	ARG	N-CA-C	-6.87	99.02	109.95
1	A	457	SER	CA-C-N	6.85	126.53	119.82
1	A	457	SER	C-N-CA	6.85	126.53	119.82
1	B	354	GLN	N-CA-C	-6.75	101.17	110.35
1	B	753	LEU	N-CA-C	6.73	118.62	111.28
1	A	276	LEU	N-CA-C	-6.69	103.91	111.07
1	A	524	ASP	N-CA-C	-6.67	106.34	114.75
1	A	449	ARG	CA-C-N	6.67	128.18	119.84
1	A	449	ARG	C-N-CA	6.67	128.18	119.84
1	A	753	LEU	N-CA-C	6.62	120.57	112.23
1	C	19	TYR	N-CA-C	6.59	116.75	108.45
1	A	861	ASP	N-CA-C	-6.50	102.80	111.96
1	B	209	THR	CA-C-N	6.49	126.46	119.78
1	B	209	THR	C-N-CA	6.49	126.46	119.78
1	C	839	ASN	CA-C-N	6.46	127.92	119.84
1	C	839	ASN	C-N-CA	6.46	127.92	119.84
1	C	250	VAL	N-CA-C	6.44	113.10	106.21
1	C	825	VAL	N-CA-C	6.44	117.39	108.89
1	C	113	PHE	N-CA-C	6.40	118.91	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	486	LYS	N-CA-C	-6.38	104.38	111.71
1	B	486	LYS	N-CA-C	-6.29	104.30	112.23
1	C	376	GLN	N-CA-C	-6.27	105.21	112.92
1	A	543	PHE	N-CA-C	-6.26	104.70	112.90
1	D	19	TYR	N-CA-C	6.25	116.53	108.34
1	C	436	VAL	N-CA-C	6.25	117.79	108.23
1	C	214	THR	N-CA-C	6.25	118.91	109.41
1	D	504	HIS	N-CA-C	-6.24	105.49	113.23
1	A	659	MET	N-CA-C	6.24	117.95	111.03
1	C	150	ASP	N-CA-C	6.22	120.41	109.96
1	D	856	ASP	N-CA-C	6.22	120.13	112.54
1	A	89	LYS	N-CA-C	-6.22	104.43	111.14
1	C	456	CYS	N-CA-C	6.21	119.31	109.81
1	A	469	GLY	N-CA-C	6.20	119.06	111.93
1	A	403	ARG	N-CA-C	-6.17	100.15	109.95
1	A	436	VAL	N-CA-C	6.14	116.72	107.75
1	C	657	GLU	N-CA-C	6.14	119.96	112.23
1	B	18	ARG	N-CA-C	-6.11	100.24	109.95
1	C	79	GLY	N-CA-C	6.10	121.95	114.69
1	D	80	LEU	N-CA-C	6.10	118.84	110.24
1	D	813	ARG	N-CA-C	6.09	120.48	111.04
1	A	134	ASP	N-CA-C	5.99	120.29	112.92
1	B	107	LYS	N-CA-C	-5.99	105.74	113.16
1	D	203	ASN	N-CA-C	-5.95	104.73	112.23
1	D	573	VAL	N-CA-C	5.94	116.72	110.72
1	C	173	GLN	N-CA-C	-5.91	106.41	113.97
1	A	295	GLU	N-CA-C	-5.85	104.98	111.36
1	A	113	PHE	N-CA-C	5.85	118.07	109.24
1	C	37	LEU	N-CA-C	-5.85	100.68	108.34
1	D	500	LYS	N-CA-C	-5.84	106.31	113.50
1	C	753	LEU	N-CA-C	5.83	117.64	111.28
1	A	144	ASP	N-CA-C	-5.82	103.43	111.28
1	A	486	LYS	N-CA-C	-5.82	105.34	113.37
1	A	405	LYS	N-CA-C	5.80	117.30	110.97
1	A	657	GLU	N-CA-C	5.77	117.24	111.07
1	D	154	SER	CA-C-N	5.77	127.05	119.84
1	D	154	SER	C-N-CA	5.77	127.05	119.84
1	D	712	VAL	N-CA-C	5.76	117.05	109.21
1	B	608	VAL	N-CA-C	5.76	117.28	111.00
1	D	200	GLU	N-CA-C	-5.76	105.75	112.89
1	B	336	ALA	N-CA-C	-5.71	104.42	111.33
1	B	665	ARG	N-CA-C	-5.70	105.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	GLU	N-CA-C	-5.70	104.97	111.07
2	G	18	DG	C2'-C3'-O3'	-5.67	102.99	111.50
1	B	493	GLN	N-CA-C	-5.66	106.37	113.28
1	B	632	ILE	N-CA-C	-5.63	105.12	110.42
1	C	294	SER	N-CA-C	-5.62	105.07	111.14
1	C	209	THR	CA-C-N	5.62	125.80	119.90
1	C	209	THR	C-N-CA	5.62	125.80	119.90
1	B	212	ILE	N-CA-C	-5.60	100.96	108.35
1	A	273	TYR	N-CA-C	5.55	118.04	111.33
1	C	885	SER	N-CA-C	-5.54	105.39	111.82
1	B	881	GLU	N-CA-C	-5.52	104.65	111.33
1	D	123	PHE	CA-C-N	5.50	126.27	120.11
1	D	123	PHE	C-N-CA	5.50	126.27	120.11
1	A	740	ALA	N-CA-C	-5.45	105.73	112.38
1	A	241	ARG	N-CA-C	-5.45	106.47	113.01
1	A	65	MET	N-CA-C	5.40	119.49	113.01
1	A	812	ASN	N-CA-C	-5.40	105.40	111.28
1	A	894	LYS	N-CA-C	5.38	117.75	111.02
1	A	824	VAL	N-CA-C	5.37	115.83	107.99
1	C	712	VAL	N-CA-C	5.37	116.31	108.58
1	B	358	VAL	N-CA-C	-5.35	105.06	112.50
1	B	457	SER	CA-C-N	5.34	126.52	119.84
1	B	457	SER	C-N-CA	5.34	126.52	119.84
1	C	755	GLU	N-CA-C	5.32	120.25	113.55
1	C	764	PHE	N-CA-C	-5.32	105.40	111.14
1	A	216	TRP	N-CA-C	5.31	116.96	108.41
1	B	72	ILE	CB-CA-C	-5.31	105.18	111.81
1	D	648	VAL	N-CA-C	-5.30	104.42	111.05
1	A	315	SER	N-CA-C	5.28	118.51	111.75
1	D	5	TYR	N-CA-C	5.28	116.73	110.19
1	D	148	VAL	N-CA-C	5.25	114.82	107.37
1	B	55	LYS	CA-C-N	5.24	125.00	119.76
1	B	55	LYS	C-N-CA	5.24	125.00	119.76
1	B	549	GLU	N-CA-C	-5.24	107.43	113.88
1	A	281	SER	N-CA-C	-5.23	105.18	112.45
1	B	180	SER	N-CA-C	5.23	117.06	111.36
1	C	18	ARG	N-CA-C	-5.23	101.17	109.59
1	D	31	VAL	N-CA-C	5.21	116.22	108.46
1	C	884	THR	N-CA-C	5.20	117.69	111.71
1	A	658	ARG	N-CA-C	5.20	119.59	112.68
1	D	333	GLN	N-CA-C	-5.18	105.71	111.36
1	C	66	ARG	N-CA-C	-5.13	105.76	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	712	VAL	N-CA-C	5.13	116.67	108.87
1	C	171	GLN	N-CA-C	5.13	116.72	111.03
1	A	14	SER	N-CA-C	5.12	116.85	109.07
1	D	771	PHE	N-CA-C	5.11	116.66	111.14
1	D	612	GLU	N-CA-C	5.09	116.61	107.80
1	A	874	LYS	N-CA-C	5.09	119.20	112.89
1	D	374	LYS	N-CA-C	-5.09	105.63	111.07
1	A	488	TYR	N-CA-C	-5.07	106.61	112.89
1	C	209	THR	N-CA-C	5.06	116.90	109.71
1	C	442	TYR	N-CA-C	-5.06	105.85	112.23
1	A	868	TYR	N-CA-C	-5.06	104.72	111.24
1	C	84	GLY	N-CA-C	5.06	116.75	111.95
1	B	391	TYR	CA-C-N	5.05	126.16	119.84
1	B	391	TYR	C-N-CA	5.05	126.16	119.84
1	A	336	ALA	N-CA-C	-5.05	106.22	112.38
1	B	737	THR	CA-C-N	5.05	124.96	119.76
1	B	737	THR	C-N-CA	5.05	124.96	119.76
2	I	5	DG	C5'-C4'-C3'	-5.05	107.33	114.90
1	B	743	LYS	N-CA-C	-5.02	105.50	110.97
1	B	456	CYS	N-CA-C	5.01	117.48	109.81
1	B	875	THR	N-CA-C	5.01	117.52	111.40
1	A	547	ARG	N-CA-C	-5.01	106.01	111.82
1	B	475	ILE	N-CA-C	-5.01	105.66	110.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7323	0	7185	572	0
1	B	7246	0	7027	550	0
1	C	7339	0	7210	490	0
1	D	7027	0	6703	654	0
2	E	370	0	205	19	0
2	G	370	0	205	34	0
2	I	370	0	205	14	0
2	K	287	0	157	11	0
3	F	282	0	158	28	0
3	H	282	0	158	20	0
3	J	282	0	158	21	0
3	L	262	0	149	18	0
4	A	43	0	0	3	0
4	B	33	0	0	2	0
4	C	32	0	0	3	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	1	0
4	I	3	0	0	0	0
4	J	1	0	0	0	0
All	All	31561	0	29520	2389	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 39.

All (2389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LEU:HD21	1:D:241:ARG:HD3	1.26	1.14
1:D:533:LEU:HD13	1:D:534:SER:H	1.05	1.12
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.32	1.12
1:C:642:ARG:HE	1:C:646:HIS:CD2	1.67	1.12
3:J:104:DG:H2''	3:J:105:DC:H5''	1.20	1.12
2:E:6:DA:H2''	2:E:7:DA:H5'	1.31	1.11
2:E:4:CTG:H5'	2:E:4:CTG:H6	1.33	1.11
1:C:231:LYS:HG2	1:C:236:GLU:HA	1.33	1.10
3:F:104:DG:H2''	3:F:105:DC:H5''	1.09	1.07
3:J:104:DG:C2'	3:J:105:DC:H5''	1.85	1.07
1:B:732:THR:HG23	1:B:733:GLN:HE21	1.20	1.05
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.36	1.04
3:F:104:DG:C2'	3:F:105:DC:H5''	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:HB1	1:A:538:LEU:HD22	1.42	1.02
1:A:839:ASN:HB2	1:A:840:PRO:HD2	1.42	1.01
1:D:785:ALA:HB1	1:D:788:ILE:HD11	1.41	1.01
1:A:642:ARG:H	1:A:646:HIS:HD2	1.07	1.01
1:D:493:GLN:HG3	1:D:494:ARG:H	1.26	1.00
1:D:815:ILE:HG22	1:D:858:ILE:HG21	1.42	1.00
1:A:362:ILE:HD13	2:E:3:DT:H5'	1.40	1.00
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.37	1.00
1:D:533:LEU:HD13	1:D:534:SER:N	1.77	0.99
1:A:153:ASN:HD22	1:A:158:ASN:HD22	1.10	0.99
1:B:85:MET:HE2	1:B:87:ASP:H	1.24	0.99
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.26	0.98
1:D:214:THR:HG22	1:D:215:GLY:H	1.26	0.97
1:C:412:LEU:HG	1:C:683:MET:HE3	1.45	0.97
1:B:164:ILE:HD13	1:B:164:ILE:H	1.25	0.97
1:C:163:SER:HB3	1:C:318:GLN:HE22	1.29	0.96
1:A:835:LEU:HD11	1:A:846:ILE:HG22	1.43	0.96
1:A:72:ILE:O	1:A:76:GLU:HG3	1.66	0.95
3:L:110:DA:H2''	3:L:111:DT:H5'	1.46	0.94
1:B:395:PHE:HB2	1:B:591:GLN:HE21	1.32	0.94
1:C:195:LYS:H	1:C:195:LYS:NZ	1.64	0.94
2:E:6:DA:H2''	2:E:7:DA:C5'	1.98	0.94
1:B:499:ILE:HD13	1:B:499:ILE:H	1.32	0.94
1:C:711:ASN:HD21	1:C:754:GLN:HE21	0.96	0.94
1:A:703:THR:HG21	1:A:707:ARG:NH1	1.83	0.92
1:D:164:ILE:H	1:D:164:ILE:HD13	1.34	0.92
1:A:836:ARG:NH1	1:A:865:TRP:HA	1.83	0.92
1:B:505:ASN:ND2	1:B:507:ASN:HD22	1.67	0.92
1:D:597:ILE:HG21	1:D:683:MET:HE1	1.51	0.92
3:F:104:DG:H2''	3:F:105:DC:C5'	1.97	0.92
1:B:217:ASN:H	1:B:274:ILE:HG21	1.35	0.91
1:B:193:ASN:HD22	1:B:196:GLU:HG2	1.33	0.91
1:B:83:LEU:H	1:B:83:LEU:HD12	1.35	0.91
1:C:137:THR:HB	1:C:328:VAL:HG21	1.50	0.91
1:D:109:ARG:NH1	1:D:142:ILE:HD11	1.85	0.91
1:A:502:ALA:O	1:A:538:LEU:HD13	1.71	0.90
1:C:392:PRO:O	1:C:587:THR:HG21	1.70	0.90
1:A:736:SER:HA	1:A:782:VAL:HB	1.53	0.90
2:K:6:DA:H2''	2:K:7:DA:H5''	1.50	0.90
1:B:863:LEU:HA	1:B:866:MET:HE3	1.53	0.90
1:B:894:LYS:HB2	1:B:894:LYS:NZ	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:110:DA:H2''	3:F:111:DT:H5'	1.54	0.89
1:A:897:LEU:H	1:A:897:LEU:HD12	1.38	0.89
1:B:668:ARG:HH11	1:B:668:ARG:HG3	1.38	0.88
2:E:12:DA:H2''	2:E:13:DG:H5'	1.52	0.88
1:B:219:GLU:HA	1:B:223:ILE:HD12	1.53	0.88
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.55	0.88
1:A:559:ARG:HH11	1:A:559:ARG:HG2	1.38	0.87
1:D:541:MET:O	1:D:544:ARG:HG2	1.74	0.87
1:D:132:PRO:HA	1:D:229:ARG:HE	1.39	0.87
1:D:198:LEU:HD11	1:D:230:ILE:HG12	1.54	0.87
1:D:481:GLN:HB3	1:D:559:ARG:HE	1.38	0.86
1:A:708:TYR:CE2	1:A:728:MET:HG3	2.11	0.86
1:A:791:TYR:HB3	1:A:801:CYS:SG	2.15	0.86
1:A:25:ARG:HB2	1:A:25:ARG:HH11	1.39	0.86
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.57	0.86
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.74	0.85
1:D:159:VAL:HG12	1:D:160:GLU:H	1.40	0.85
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.42	0.85
1:B:115:ILE:HG22	1:B:136:ILE:HG23	1.58	0.85
1:B:745:LEU:O	1:B:749:ILE:HG13	1.77	0.85
1:C:642:ARG:NH1	1:C:646:HIS:HB3	1.92	0.84
1:B:894:LYS:HB2	1:B:894:LYS:HZ2	1.40	0.84
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.57	0.84
1:C:855:THR:HG22	1:C:857:LEU:H	1.43	0.84
1:A:127:SER:HA	1:A:228:ASN:ND2	1.92	0.84
1:B:271:LEU:HB3	1:B:276:LEU:HD11	1.59	0.84
2:E:5:DG:H2''	2:E:6:DA:OP2	1.78	0.83
1:D:10:GLN:HA	1:D:15:ILE:HG22	1.59	0.83
1:D:814:ALA:HB3	1:D:841:PHE:CE1	2.13	0.83
2:I:4:CTG:H5''	2:I:4:CTG:H6	1.61	0.83
1:B:777:ILE:HD11	1:B:853:GLU:HG2	1.58	0.83
3:L:104:DG:H2''	3:L:105:DC:C5'	2.09	0.83
2:K:6:DA:H2''	2:K:7:DA:C5'	2.07	0.83
1:D:686:GLU:HB3	1:D:715:MET:HE1	1.61	0.83
1:A:2:LYS:HA	1:A:2:LYS:NZ	1.94	0.82
1:A:43:GLU:H	1:A:43:GLU:CD	1.87	0.82
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.42	0.82
1:B:508:LEU:HD23	1:B:508:LEU:H	1.44	0.82
1:D:133:ILE:HG12	1:D:229:ARG:HD2	1.62	0.82
1:D:212:ILE:HD11	1:D:345:LEU:HD21	1.62	0.82
1:D:503:LEU:HD11	1:D:539:ASN:HD22	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:HG22	1:B:265:LEU:HA	1.62	0.82
1:A:836:ARG:HH11	1:A:865:TRP:HA	1.44	0.81
1:D:61:LEU:HD23	1:D:62:PHE:N	1.94	0.81
1:C:836:ARG:HH12	1:C:865:TRP:HA	1.44	0.81
3:L:104:DG:H2''	3:L:105:DC:H5''	1.62	0.81
1:B:818:ASN:ND2	1:B:821:ALA:HB2	1.95	0.81
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.61	0.81
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.62	0.81
1:A:347:MET:HA	1:A:347:MET:HE3	1.62	0.81
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.62	0.81
1:D:164:ILE:HG21	1:D:186:ILE:CD1	2.11	0.81
1:A:236:GLU:HG2	1:A:240:LYS:HE2	1.60	0.81
1:A:546:GLN:C	1:A:546:GLN:HE21	1.88	0.81
1:C:295:GLU:OE1	1:C:301:GLY:HA2	1.81	0.81
1:A:642:ARG:H	1:A:646:HIS:CD2	1.97	0.80
1:C:818:ASN:ND2	1:C:857:LEU:HD11	1.96	0.80
1:D:803:PHE:HB2	2:K:11:DC:H4'	1.62	0.80
1:D:843:ASP:OD1	1:D:844:LYS:HD3	1.82	0.80
1:A:2:LYS:HA	1:A:2:LYS:HZ3	1.46	0.80
1:A:544:ARG:HB2	1:A:544:ARG:HH11	1.45	0.80
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.63	0.80
1:D:164:ILE:HG21	1:D:186:ILE:HD12	1.63	0.80
1:D:444:ASN:HA	1:D:599:ARG:NH1	1.96	0.80
1:D:495:ASN:HD22	1:D:521:ASP:HA	1.43	0.80
1:D:597:ILE:O	1:D:601:VAL:HG23	1.81	0.80
1:A:303:LEU:HD12	1:A:323:TYR:HA	1.64	0.80
1:D:140:ASP:HB3	1:D:143:ASP:HB3	1.62	0.80
1:B:658:ARG:HG2	1:D:897:LEU:HD21	1.63	0.80
1:D:793:VAL:HG22	1:D:796:PHE:O	1.82	0.80
1:B:808:ILE:HG22	1:B:812:ASN:HD21	1.45	0.80
1:A:422:GLN:NE2	1:A:680:LEU:H	1.79	0.79
1:B:27:ARG:HH11	1:B:27:ARG:HG3	1.47	0.79
1:D:533:LEU:CD1	1:D:534:SER:H	1.93	0.79
1:B:797:PRO:HG3	1:B:806:ARG:NH1	1.97	0.79
1:D:214:THR:HG22	1:D:215:GLY:N	1.96	0.79
1:D:398:GLU:HA	1:D:705:LYS:HE3	1.63	0.79
1:A:362:ILE:HG12	1:A:572:ASN:ND2	1.97	0.79
1:B:499:ILE:HD13	1:B:499:ILE:N	1.96	0.79
1:D:109:ARG:HB2	1:D:211:VAL:HG23	1.63	0.79
1:D:818:ASN:OD1	1:D:855:THR:HG21	1.82	0.79
1:A:25:ARG:HB2	1:A:25:ARG:NH1	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TRP:HA	1:B:318:GLN:HE22	1.46	0.79
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.17	0.79
1:D:493:GLN:HG3	1:D:494:ARG:N	1.93	0.79
1:C:686:GLU:HG3	1:C:715:MET:CE	2.13	0.79
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.64	0.78
1:A:653:LYS:HD3	1:A:657:GLU:CD	2.07	0.78
1:B:800:LYS:HD3	3:H:108:DT:H4'	1.62	0.78
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.63	0.78
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.65	0.78
1:C:195:LYS:H	1:C:195:LYS:HZ3	1.31	0.78
1:B:534:SER:OG	1:B:537:SER:HB2	1.82	0.78
1:C:73:LYS:NZ	1:C:73:LYS:HB3	1.97	0.78
1:C:642:ARG:N	1:C:642:ARG:HD3	1.99	0.78
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.65	0.78
3:F:106:DT:H1'	3:F:107:DG:H5'	1.66	0.78
1:A:127:SER:HA	1:A:228:ASN:HD22	1.48	0.77
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.65	0.77
1:B:505:ASN:HD22	1:B:507:ASN:HD22	1.32	0.77
1:C:642:ARG:NE	1:C:646:HIS:CD2	2.51	0.77
1:D:132:PRO:HA	1:D:229:ARG:NE	1.99	0.77
3:J:104:DG:H2''	3:J:105:DC:C5'	2.10	0.77
1:A:246:ARG:HG2	1:A:246:ARG:HH11	1.48	0.77
1:D:150:ASP:HB3	1:D:188:TYR:HE1	1.48	0.77
1:D:598:GLU:CG	1:D:617:VAL:HG21	2.14	0.77
1:C:726:LYS:HE2	1:C:728:MET:HE3	1.67	0.77
1:B:151:LEU:HA	1:B:191:PHE:O	1.84	0.77
1:B:322:SER:O	1:B:326:ILE:HG12	1.85	0.77
1:D:494:ARG:O	1:D:497:GLU:HG2	1.85	0.77
2:E:4:CTG:O6	2:E:4:CTG:H2'	1.84	0.77
2:K:6:DA:C2'	2:K:7:DA:H5''	2.15	0.77
1:D:182:ILE:O	1:D:182:ILE:HD13	1.86	0.77
1:B:218:VAL:O	1:B:223:ILE:HG13	1.84	0.76
1:B:751:ARG:HH11	1:B:759:SER:HB3	1.49	0.76
1:B:222:ALA:O	1:B:226:VAL:HG23	1.83	0.76
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.67	0.76
1:D:849:PRO:HG2	1:D:852:THR:OG1	1.85	0.76
2:I:6:DA:H2''	2:I:7:DA:H5'	1.67	0.76
1:C:373:LEU:HB3	1:C:378:LYS:HB2	1.66	0.76
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.68	0.76
1:B:818:ASN:HD22	1:B:821:ALA:HB2	1.47	0.76
1:A:25:ARG:HH11	1:A:25:ARG:CB	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PHE:CE2	1:C:68:ALA:HA	2.21	0.76
1:C:836:ARG:NH1	1:C:865:TRP:HA	2.01	0.76
1:D:305:TYR:OH	1:D:312:LEU:HB2	1.85	0.76
1:D:815:ILE:HG21	1:D:858:ILE:HD13	1.68	0.76
3:J:105:DC:H2'	3:J:106:DT:H71	1.68	0.75
1:C:482:ARG:HH12	1:C:556:GLN:HE21	1.32	0.75
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.67	0.75
2:I:4:CTG:H5''	2:I:4:CTG:C6	2.16	0.75
1:D:407:VAL:HG13	1:D:689:ALA:HB3	1.68	0.75
1:C:85:MET:HA	1:C:380:ILE:HD11	1.69	0.75
3:L:110:DA:H2''	3:L:111:DT:C5'	2.16	0.75
1:A:428:GLU:N	1:A:428:GLU:OE2	2.20	0.75
1:A:139:TYR:CE2	1:A:332:LEU:HD21	2.21	0.75
1:C:752:MET:HE3	1:C:889:LEU:HD12	1.68	0.75
1:A:384:ARG:HD3	1:A:385:SER:N	2.02	0.74
1:B:166:ILE:HD12	1:B:166:ILE:H	1.51	0.74
1:B:854:ILE:HD11	1:B:858:ILE:HG13	1.68	0.74
1:C:195:LYS:HZ3	1:C:195:LYS:N	1.84	0.74
1:D:738:PRO:HB3	1:D:780:ALA:O	1.87	0.74
1:D:512:GLU:CB	1:D:513:PRO:HA	2.17	0.74
1:A:153:ASN:HD22	1:A:158:ASN:ND2	1.83	0.74
1:A:847:ALA:O	1:A:848:TRP:HB3	1.86	0.74
1:C:216:TRP:O	1:C:217:ASN:HB2	1.87	0.74
1:D:856:ASP:HA	1:D:859:LYS:HB2	1.68	0.74
1:D:835:LEU:O	1:D:835:LEU:HD12	1.87	0.74
1:B:775:ASN:HD21	1:B:777:ILE:HB	1.53	0.74
1:D:202:LEU:CD2	1:D:241:ARG:HD3	2.11	0.74
1:A:404:TYR:CD1	1:A:618:LEU:HD13	2.23	0.74
1:D:82:ALA:N	1:D:382:GLN:HE21	1.86	0.74
1:C:231:LYS:HG2	1:C:236:GLU:CA	2.16	0.74
1:D:97:TYR:HB3	1:D:101:ILE:HD11	1.67	0.74
1:A:171:GLN:HE22	1:A:319:ARG:HH12	1.35	0.73
1:A:636:VAL:O	1:A:640:LYS:HD2	1.88	0.73
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.67	0.73
1:D:117:VAL:HG13	1:D:132:PRO:O	1.88	0.73
1:A:818:ASN:HD22	1:A:857:LEU:HD11	1.54	0.73
2:E:8:DT:H2'	2:E:9:DG:C8	2.23	0.73
2:K:10:DA:H2''	2:K:11:DC:H5'	1.70	0.73
1:D:229:ARG:NH1	1:D:233:ILE:HD11	2.04	0.73
1:D:441:ASP:HB3	1:D:447:ALA:HB2	1.70	0.73
1:B:193:ASN:ND2	1:B:196:GLU:HG2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ARG:HD3	1:C:642:ARG:H	1.50	0.73
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.70	0.73
1:B:516:VAL:HG13	1:B:544:ARG:HH11	1.52	0.73
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.70	0.73
1:D:81:GLU:OE2	1:D:83:LEU:HD21	1.89	0.73
1:C:180:SER:O	1:C:183:ILE:HG22	1.88	0.73
1:A:392:PRO:O	1:A:587:THR:HG21	1.89	0.73
1:B:83:LEU:HD12	1:B:83:LEU:N	2.03	0.73
1:C:163:SER:HB3	1:C:318:GLN:NE2	2.04	0.73
1:A:501:GLU:HA	1:A:504:HIS:ND1	2.04	0.72
3:H:106:DT:H1'	3:H:107:DG:H5'	1.71	0.72
1:A:482:ARG:HH21	1:A:556:GLN:HE22	1.36	0.72
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.02	0.72
1:B:408:MET:HE2	1:B:685:ARG:HD3	1.70	0.72
1:C:73:LYS:HB3	1:C:73:LYS:HZ3	1.55	0.72
1:B:446:VAL:HG22	1:B:446:VAL:O	1.87	0.72
1:C:109:ARG:NH1	1:C:208:LYS:HA	2.03	0.72
1:D:62:PHE:HB3	1:D:67:ASP:OD1	1.89	0.72
1:D:204:PHE:CE1	1:D:208:LYS:HG3	2.25	0.72
1:A:862:VAL:O	1:A:864:HIS:N	2.23	0.72
1:D:140:ASP:OD1	1:D:142:ILE:HG12	1.89	0.72
1:A:808:ILE:O	1:A:811:TYR:HB3	1.90	0.72
1:B:217:ASN:OD1	1:B:274:ILE:HD13	1.90	0.72
1:A:64:ASN:C	1:A:64:ASN:HD22	1.97	0.72
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.70	0.72
1:D:222:ALA:O	1:D:226:VAL:HG23	1.89	0.72
1:D:398:GLU:CA	1:D:705:LYS:HE3	2.19	0.72
1:D:326:ILE:O	1:D:330:ARG:HG2	1.90	0.72
1:B:71:TRP:CZ2	1:B:75:MET:HE3	2.25	0.71
1:B:621:ASP:OD1	3:H:114:DA:H5'	1.90	0.71
1:B:749:ILE:HG22	1:B:753:LEU:HD12	1.70	0.71
1:D:802:PRO:HD2	1:D:805:ILE:HD12	1.72	0.71
3:J:104:DG:C3'	3:J:105:DC:H5''	2.19	0.71
1:A:153:ASN:ND2	1:A:158:ASN:HD22	1.85	0.71
1:B:781:SER:HB2	1:B:832:VAL:HB	1.72	0.71
1:D:495:ASN:ND2	1:D:521:ASP:HA	2.05	0.71
2:G:14:DC:H2''	2:G:15:DC:H5''	1.73	0.71
1:B:347:MET:CE	1:B:562:LEU:HD11	2.21	0.71
1:A:40:HIS:HD2	1:A:57:CYS:SG	2.14	0.71
1:A:818:ASN:ND2	1:A:857:LEU:HD11	2.05	0.71
1:A:279:LYS:HZ2	2:E:3:DT:H71	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LYS:HE3	3:F:113:DC:O2	1.91	0.71
1:C:109:ARG:HH12	1:C:208:LYS:CD	2.04	0.71
1:C:322:SER:O	1:C:326:ILE:HG13	1.90	0.71
1:C:656:ARG:HA	1:C:660:GLU:HG3	1.73	0.71
1:D:434:PHE:CE1	1:D:460:GLY:HA2	2.26	0.71
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.18	0.71
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.05	0.71
2:I:10:DA:H2''	2:I:11:DC:H5'	1.72	0.71
1:B:517:ASP:OD1	1:B:519:ARG:HB2	1.91	0.70
1:C:176:ASP:OD2	1:C:319:ARG:HD3	1.89	0.70
1:C:272:ASP:OD1	1:C:274:ILE:HG22	1.90	0.70
1:D:846:ILE:HD11	1:D:862:VAL:HG11	1.71	0.70
1:D:504:HIS:C	1:D:506:PRO:HD3	2.14	0.70
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.72	0.70
1:D:322:SER:O	1:D:326:ILE:HG12	1.90	0.70
1:D:535:ALA:HB1	1:D:539:ASN:ND2	2.05	0.70
1:D:109:ARG:NH2	1:D:208:LYS:HB3	2.06	0.70
1:C:183:ILE:HD12	1:C:186:ILE:HD12	1.72	0.70
1:D:109:ARG:HH11	1:D:142:ILE:HD11	1.55	0.70
1:A:707:ARG:NH2	1:A:731:GLU:OE1	2.25	0.70
1:B:732:THR:CG2	1:B:733:GLN:HE21	2.02	0.70
1:D:41:CYS:HB3	1:D:57:CYS:HA	1.72	0.70
1:B:312:LEU:HD13	1:B:312:LEU:O	1.92	0.70
1:B:811:TYR:OH	1:B:822:PRO:HG2	1.91	0.70
1:C:711:ASN:HD21	1:C:754:GLN:NE2	1.81	0.70
1:A:536:LYS:O	1:A:536:LYS:HD3	1.92	0.70
1:B:408:MET:CE	1:B:685:ARG:HD3	2.22	0.70
1:D:685:ARG:HD2	1:D:685:ARG:C	2.17	0.70
1:C:587:THR:HG22	1:C:588:THR:N	2.05	0.70
1:A:485:HIS:C	1:A:487:GLY:H	1.98	0.70
1:A:514:LEU:HD12	1:A:526:ILE:HG23	1.73	0.70
1:A:642:ARG:HB2	1:A:642:ARG:NH1	2.07	0.70
1:C:13:ASP:OD2	1:C:66:ARG:HB2	1.91	0.70
1:B:785:ALA:HB1	1:B:788:ILE:HD11	1.74	0.69
1:A:362:ILE:CD1	1:A:572:ASN:HD22	2.05	0.69
1:D:85:MET:HE3	1:D:90:LEU:HD22	1.74	0.69
1:A:384:ARG:HD3	1:A:385:SER:H	1.56	0.69
1:B:164:ILE:HD13	1:B:164:ILE:N	2.05	0.69
1:B:875:THR:O	1:B:879:PRO:HG3	1.92	0.69
1:D:82:ALA:HB3	1:D:382:GLN:HG3	1.75	0.69
1:D:114:ASP:HB3	1:D:328:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.25	0.69
1:B:326:ILE:O	1:B:330:ARG:HG2	1.92	0.69
1:C:176:ASP:O	1:C:177:GLU:HB2	1.91	0.69
2:E:12:DA:H2''	2:E:13:DG:C5'	2.22	0.69
1:B:204:PHE:HE1	1:B:208:LYS:HD2	1.57	0.69
1:D:330:ARG:O	1:D:334:ILE:HG13	1.92	0.69
1:A:335:ASP:OD2	1:A:341:ILE:HG12	1.92	0.69
1:D:204:PHE:O	1:D:208:LYS:HG2	1.92	0.69
1:C:655:ALA:O	1:C:660:GLU:HG2	1.93	0.69
1:D:6:LEU:HB2	1:D:18:ARG:O	1.93	0.69
1:A:606:ASN:HD21	1:A:613:GLY:N	1.91	0.69
1:B:732:THR:HG23	1:B:733:GLN:NE2	2.03	0.69
1:C:382:GLN:HG2	1:C:383:GLY:N	2.07	0.69
1:D:149:PHE:HB3	1:D:197:LEU:CD2	2.21	0.69
1:D:234:PHE:HB3	1:D:238:THR:HB	1.74	0.69
1:D:761:GLN:HG2	1:D:891:TYR:C	2.18	0.69
2:I:16:DG:H2''	2:I:17:DC:O5'	1.92	0.69
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.75	0.69
1:D:201:TYR:O	1:D:204:PHE:HB3	1.92	0.69
1:A:474:GLU:O	1:A:478:VAL:HG23	1.92	0.69
1:C:524:ASP:HA	1:C:527:LYS:HE2	1.75	0.68
1:D:811:TYR:HA	1:D:841:PHE:CZ	2.27	0.68
1:C:354:GLN:HB3	1:C:356:GLN:OE1	1.93	0.68
1:D:214:THR:CG2	1:D:215:GLY:H	2.04	0.68
1:A:606:ASN:HD21	1:A:613:GLY:CA	2.05	0.68
1:D:373:LEU:HD12	1:D:380:ILE:HG22	1.75	0.68
1:A:43:GLU:CD	1:A:43:GLU:N	2.52	0.68
1:C:482:ARG:NH1	1:C:560:LYS:HB2	2.08	0.68
1:B:217:ASN:H	1:B:274:ILE:CG2	2.05	0.68
1:C:14:SER:OG	1:C:30:GLU:HG2	1.92	0.68
1:C:449:ARG:HH12	1:C:452:ASP:HA	1.58	0.68
1:D:147:TYR:HA	1:D:187:ILE:HG23	1.76	0.68
1:D:777:ILE:O	1:D:777:ILE:HG22	1.94	0.68
1:D:159:VAL:HG11	1:D:317:HIS:CB	2.24	0.68
1:D:159:VAL:HG11	1:D:317:HIS:HB3	1.76	0.68
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.75	0.68
1:C:791:TYR:CE2	1:C:802:PRO:HD3	2.28	0.68
1:D:132:PRO:CA	1:D:229:ARG:HH21	2.07	0.68
1:D:864:HIS:C	1:D:866:MET:H	2.01	0.68
1:A:308:PRO:HG2	1:A:311:LYS:HG2	1.74	0.67
1:A:466:ASP:OD2	1:A:467:ARG:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:ARG:HG3	1:D:658:ARG:HH11	1.57	0.67
1:B:6:LEU:HG	1:B:19:TYR:HA	1.76	0.67
1:D:293:ILE:HD12	1:D:294:SER:N	2.10	0.67
1:A:835:LEU:HD21	1:A:846:ILE:CG2	2.25	0.67
1:C:145:ARG:HB2	1:C:147:TYR:HE1	1.60	0.67
1:C:188:TYR:O	1:C:189:MET:HG3	1.94	0.67
1:D:214:THR:CG2	1:D:273:TYR:HB2	2.24	0.67
1:A:502:ALA:CB	1:A:538:LEU:HD22	2.23	0.67
1:A:621:ASP:OD2	3:F:114:DA:H5'	1.95	0.67
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.77	0.67
1:B:641:PHE:HA	1:B:646:HIS:HD2	1.58	0.67
1:D:775:ASN:HB3	1:D:778:SER:OG	1.95	0.67
1:D:797:PRO:HG2	1:D:806:ARG:NH1	2.09	0.67
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.25	0.67
1:A:824:VAL:HG13	1:A:849:PRO:HG3	1.76	0.67
1:B:553:MET:O	1:B:557:ILE:HG12	1.94	0.67
1:C:28:THR:HG23	1:C:28:THR:O	1.95	0.67
1:C:170:LEU:HD23	1:C:177:GLU:HG2	1.77	0.67
1:D:509:SER:HB2	1:D:532:LYS:O	1.95	0.67
1:A:544:ARG:HB2	1:A:544:ARG:NH1	2.10	0.67
1:C:221:PHE:O	1:C:224:PRO:HD2	1.94	0.67
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.58	0.67
1:B:98:ASN:O	1:B:99:TYR:HB3	1.94	0.67
1:B:134:ASP:OD1	1:B:151:LEU:HB3	1.95	0.67
1:B:483:LYS:O	1:B:486:LYS:HG2	1.95	0.67
1:B:766:GLU:HG3	1:B:767:PHE:N	2.09	0.67
3:F:101:DG:H2''	3:F:102:DC:O5'	1.95	0.67
2:G:4:CTG:H6	2:G:4:CTG:H5''	1.76	0.67
2:G:16:DG:H2''	2:G:17:DC:H5''	1.77	0.67
1:A:347:MET:HB2	1:A:558:ASN:OD1	1.94	0.66
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.60	0.66
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.25	0.66
1:D:159:VAL:HG12	1:D:160:GLU:N	2.08	0.66
1:B:499:ILE:HG12	1:B:542:LEU:HD13	1.77	0.66
1:D:505:ASN:N	1:D:506:PRO:HD3	2.10	0.66
1:D:533:LEU:CD1	1:D:534:SER:N	2.55	0.66
1:D:561:LEU:O	1:D:561:LEU:HD23	1.96	0.66
1:B:700:GLY:HA2	1:B:753:LEU:HD21	1.76	0.66
1:C:154:SER:C	1:C:156:TYR:H	2.01	0.66
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.60	0.66
1:B:216:TRP:HA	1:B:274:ILE:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLN:CB	1:D:559:ARG:HE	2.08	0.66
1:A:83:LEU:N	1:A:83:LEU:HD12	2.10	0.66
1:B:351:ALA:O	1:B:352:LYS:HB2	1.94	0.66
1:B:102:LYS:HD2	1:B:103:TYR:H	1.60	0.66
1:B:599:ARG:HG2	1:B:599:ARG:HH11	1.60	0.66
1:B:728:MET:HG3	3:H:113:DC:H5'	1.78	0.66
1:D:281:SER:HB3	1:D:283:THR:HG22	1.78	0.66
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.77	0.66
1:A:840:PRO:C	1:A:842:GLY:H	2.04	0.66
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.30	0.66
1:C:193:ASN:HD22	1:C:195:LYS:NZ	1.94	0.66
1:A:730:LEU:HB3	1:A:883:PHE:CZ	2.31	0.66
1:B:253:ILE:HD12	1:B:254:GLU:H	1.59	0.66
1:D:15:ILE:HD11	1:D:92:TYR:CD2	2.31	0.66
3:H:110:DA:H2''	3:H:111:DT:C5'	2.26	0.66
1:A:712:VAL:HG22	1:A:724:LYS:O	1.96	0.65
1:B:326:ILE:HG23	1:B:330:ARG:CZ	2.26	0.65
1:B:749:ILE:HG22	1:B:753:LEU:CD1	2.26	0.65
1:B:186:ILE:HG22	1:B:187:ILE:N	2.11	0.65
1:C:439:LEU:HD12	1:C:443:ILE:HD11	1.78	0.65
1:C:757:GLU:HB2	1:C:889:LEU:HD22	1.76	0.65
1:A:403:ARG:HD2	1:A:887:ALA:O	1.96	0.65
1:C:130:LYS:HE3	1:C:131:HIS:CE1	2.29	0.65
1:D:396:VAL:HB	2:K:7:DA:OP1	1.97	0.65
1:D:517:ASP:OD1	1:D:519:ARG:HG2	1.96	0.65
3:J:110:DA:H2''	3:J:111:DT:C5'	2.27	0.65
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.25	0.65
1:D:151:LEU:HD11	1:D:154:SER:OG	1.97	0.65
1:D:112:ASN:HB3	1:D:214:THR:HB	1.77	0.65
3:L:104:DG:H2''	3:L:105:DC:H5'	1.79	0.65
1:A:203:ASN:O	1:A:207:GLN:HG2	1.97	0.65
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.31	0.65
1:C:465:LYS:HZ2	1:C:675:ASN:HD21	1.45	0.65
1:D:216:TRP:CZ2	1:D:293:ILE:HG12	2.32	0.65
1:D:594:LEU:O	1:D:597:ILE:HG22	1.96	0.65
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.26	0.65
1:C:109:ARG:HH12	1:C:208:LYS:HD3	1.62	0.65
1:D:469:GLY:C	1:D:472:PRO:HD2	2.22	0.65
1:D:813:ARG:HG3	1:D:814:ALA:H	1.60	0.65
1:A:71:TRP:CZ3	1:A:82:ALA:HB1	2.32	0.65
1:B:347:MET:HE1	1:B:350:TYR:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:CE2	1:D:201:TYR:HA	2.32	0.65
1:C:81:GLU:HB2	1:C:384:ARG:HH22	1.60	0.64
1:C:818:ASN:HB2	4:C:921:HOH:O	1.97	0.64
1:D:598:GLU:HG2	1:D:617:VAL:HG21	1.78	0.64
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.13	0.64
1:A:396:VAL:HG22	1:A:621:ASP:OD1	1.98	0.64
1:B:777:ILE:CD1	1:B:853:GLU:HG2	2.27	0.64
1:D:604:TYR:O	1:D:608:VAL:HG23	1.97	0.64
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.77	0.64
1:C:114:ASP:HB3	1:C:328:VAL:HG22	1.77	0.64
3:F:102:DC:H2''	3:F:103:DG:OP2	1.96	0.64
2:G:11:DC:H2''	2:G:12:DA:H5'	1.78	0.64
1:A:862:VAL:C	1:A:864:HIS:H	2.04	0.64
1:B:668:ARG:HG3	1:B:668:ARG:NH1	2.07	0.64
1:C:10:GLN:HG3	1:C:65:MET:HE1	1.79	0.64
1:C:147:TYR:HB3	1:C:149:PHE:HE1	1.62	0.64
1:C:686:GLU:HG3	1:C:715:MET:HE1	1.79	0.64
1:D:783:SER:HA	3:L:111:DT:OP1	1.97	0.64
1:A:501:GLU:HA	1:A:504:HIS:HD1	1.62	0.64
1:C:153:ASN:HB2	1:C:192:ASP:O	1.98	0.64
1:B:501:GLU:HG3	1:B:501:GLU:O	1.96	0.64
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.33	0.64
1:A:540:GLU:O	1:A:544:ARG:HD3	1.98	0.64
1:B:636:VAL:O	1:B:640:LYS:HG3	1.97	0.64
1:C:271:LEU:HB3	1:C:276:LEU:CD2	2.28	0.64
1:D:164:ILE:H	1:D:164:ILE:CD1	2.11	0.64
1:D:355:ILE:O	1:D:358:VAL:HG23	1.96	0.64
1:A:621:ASP:O	3:F:114:DA:H4'	1.97	0.64
1:D:78:ILE:O	1:D:78:ILE:HG22	1.98	0.64
1:A:470:VAL:O	1:A:474:GLU:HG2	1.98	0.64
1:B:338:ARG:O	1:B:339:GLN:HB2	1.96	0.64
1:D:163:SER:HB2	1:D:166:ILE:CD1	2.28	0.64
2:G:14:DC:C2'	2:G:15:DC:H5''	2.28	0.64
1:B:362:ILE:HD11	1:B:572:ASN:HB3	1.80	0.64
1:C:302:LYS:HA	1:C:302:LYS:HE3	1.78	0.64
1:A:555:ALA:HB1	1:A:559:ARG:HH12	1.62	0.63
1:B:76:GLU:HG2	1:B:382:GLN:HE22	1.63	0.63
1:B:164:ILE:H	1:B:164:ILE:CD1	2.00	0.63
1:B:641:PHE:HA	1:B:646:HIS:CD2	2.33	0.63
1:C:120:PRO:HD2	1:C:131:HIS:HE2	1.64	0.63
1:C:330:ARG:O	1:C:333:GLN:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:LYS:NZ	1:C:675:ASN:HD21	1.96	0.63
1:D:116:GLU:HB3	1:D:320:TYR:OH	1.98	0.63
1:D:767:PHE:O	1:D:771:PHE:HB2	1.97	0.63
1:A:439:LEU:O	1:A:443:ILE:HG13	1.98	0.63
1:C:187:ILE:O	1:C:187:ILE:HG22	1.97	0.63
1:C:270:VAL:O	1:C:271:LEU:HD23	1.99	0.63
1:C:524:ASP:HA	1:C:527:LYS:CE	2.28	0.63
2:E:4:CTG:H5'	2:E:4:CTG:C6	2.22	0.63
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.80	0.63
1:B:401:PRO:O	1:B:402:ASN:HB2	1.98	0.63
1:C:642:ARG:H	1:C:642:ARG:CD	2.11	0.63
1:D:125:GLU:HG3	1:D:127:SER:H	1.62	0.63
1:D:171:GLN:OE1	1:D:303:LEU:HD11	1.98	0.63
1:A:708:TYR:CZ	1:A:728:MET:HG3	2.33	0.63
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.29	0.63
1:B:334:ILE:O	1:B:338:ARG:HG2	1.99	0.63
1:C:382:GLN:HG2	1:C:383:GLY:H	1.61	0.63
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.79	0.63
1:C:204:PHE:CE1	1:C:208:LYS:HG3	2.33	0.63
1:D:21:ASP:HB2	1:D:23:ASN:OD1	1.98	0.63
1:D:189:MET:HB3	1:D:191:PHE:CZ	2.34	0.63
1:B:117:VAL:HG21	1:B:225:TYR:CE2	2.34	0.63
1:C:422:GLN:HG3	1:C:678:GLN:O	1.99	0.63
1:C:791:TYR:CD2	1:C:802:PRO:HD3	2.34	0.63
1:A:559:ARG:HH11	1:A:559:ARG:CG	2.10	0.63
1:A:276:LEU:HD21	1:A:341:ILE:HD13	1.79	0.63
1:A:836:ARG:HG3	1:A:867:ASP:HA	1.80	0.63
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.34	0.63
1:D:183:ILE:O	1:D:186:ILE:HG12	1.99	0.63
1:C:6:LEU:HD13	1:C:211:VAL:HG21	1.81	0.62
1:D:219:GLU:OE1	1:D:262:ILE:HD13	1.99	0.62
1:D:444:ASN:HA	1:D:599:ARG:HH11	1.62	0.62
1:D:605:LEU:HD22	1:D:632:ILE:HD11	1.80	0.62
2:K:8:DT:H2''	2:K:9:DG:C8	2.34	0.62
1:A:239:ALA:O	1:A:242:LEU:HB2	1.99	0.62
1:B:740:ALA:HB2	1:B:778:SER:HB2	1.81	0.62
2:G:6:DA:H2''	2:G:7:DA:C5'	2.28	0.62
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.33	0.62
1:B:470:VAL:O	1:B:474:GLU:HB2	1.99	0.62
1:D:170:LEU:HD22	1:D:177:GLU:HG2	1.79	0.62
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:110:DA:H2''	3:J:111:DT:H5'	1.80	0.62
1:B:273:TYR:OH	1:B:340:PHE:HB2	2.00	0.62
1:C:787:ASN:HD22	1:C:790:LYS:HD2	1.64	0.62
1:D:713:TRP:CZ3	1:D:723:PRO:HD3	2.33	0.62
1:C:167:ALA:O	1:C:176:ASP:HB2	2.00	0.62
1:D:7:THR:HG21	1:D:267:GLY:O	2.00	0.62
1:B:837:GLU:HG2	1:B:838:GLY:N	2.14	0.62
1:C:195:LYS:NZ	1:C:195:LYS:N	2.39	0.62
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.34	0.62
1:A:362:ILE:HD11	1:A:569:ALA:HA	1.81	0.62
1:A:467:ARG:HG3	1:A:467:ARG:HH11	1.64	0.62
1:A:810:THR:HG22	1:A:841:PHE:HB3	1.82	0.62
1:C:540:GLU:O	1:C:544:ARG:HG3	2.00	0.62
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.81	0.62
1:A:499:ILE:HB	1:A:542:LEU:HD13	1.80	0.62
1:B:85:MET:HE2	1:B:87:ASP:N	2.08	0.62
1:D:247:LYS:O	1:D:266:PHE:HB2	1.99	0.62
1:D:294:SER:HB3	1:D:300:VAL:HG21	1.80	0.62
1:C:839:ASN:OD1	1:C:841:PHE:HB2	1.99	0.62
1:D:90:LEU:HD12	1:D:363:LYS:HE3	1.81	0.62
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.35	0.62
1:B:171:GLN:NE2	1:B:303:LEU:HD13	2.15	0.62
1:B:681:MET:HA	1:B:681:MET:HE2	1.82	0.62
1:C:365:TRP:CE2	1:C:566:LEU:HD13	2.34	0.62
1:D:725:LEU:HD13	1:D:725:LEU:H	1.65	0.62
1:A:218:VAL:HG23	1:A:222:ALA:HB3	1.81	0.61
1:B:221:PHE:C	1:B:224:PRO:HD2	2.25	0.61
1:B:499:ILE:CG1	1:B:542:LEU:HD13	2.30	0.61
1:D:313:ARG:HG3	1:D:317:HIS:HD2	1.65	0.61
1:D:707:ARG:HA	1:D:729:GLY:HA3	1.82	0.61
1:D:736:SER:HA	1:D:782:VAL:HB	1.82	0.61
1:D:750:ARG:HH11	1:D:754:GLN:NE2	1.97	0.61
2:I:4:CTG:H6	2:I:4:CTG:C5'	2.29	0.61
1:A:726:LYS:HG3	1:A:728:MET:HE3	1.82	0.61
1:B:129:ALA:HB1	1:B:229:ARG:HG2	1.82	0.61
1:B:319:ARG:O	1:B:323:TYR:HB2	2.00	0.61
1:A:362:ILE:HD13	2:E:3:DT:C5'	2.24	0.61
1:A:656:ARG:HA	1:A:660:GLU:HG3	1.83	0.61
1:B:82:ALA:O	1:B:382:GLN:HB2	2.00	0.61
1:C:97:TYR:O	1:C:352:LYS:HE2	2.00	0.61
1:D:576:ARG:NH1	1:D:576:ARG:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:TYR:CB	1:D:846:ILE:HB	2.30	0.61
1:A:745:LEU:HD13	1:A:876:PHE:HD1	1.65	0.61
1:B:233:ILE:HD12	1:B:233:ILE:N	2.15	0.61
1:C:455:SER:OG	1:C:676:ASN:HA	1.99	0.61
1:D:818:ASN:OD1	1:D:857:LEU:HD12	2.01	0.61
3:F:110:DA:H2''	3:F:111:DT:C5'	2.28	0.61
1:A:280:PHE:N	1:A:280:PHE:CD1	2.66	0.61
1:B:797:PRO:HG3	1:B:806:ARG:HH12	1.65	0.61
1:C:514:LEU:HD21	1:C:526:ILE:HG23	1.82	0.61
1:C:775:ASN:OD1	1:C:777:ILE:N	2.30	0.61
1:D:198:LEU:HD13	1:D:198:LEU:O	2.00	0.61
1:D:441:ASP:O	1:D:446:VAL:HG12	2.00	0.61
1:D:725:LEU:HD13	1:D:725:LEU:N	2.15	0.61
2:G:4:CTG:H6	2:G:4:CTG:C5'	2.31	0.61
1:B:685:ARG:HG2	1:B:685:ARG:HH11	1.66	0.61
1:D:575:PHE:HE2	1:D:577:TYR:HB2	1.65	0.61
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.82	0.61
1:A:410:PHE:N	1:A:410:PHE:CD1	2.68	0.61
1:B:468:ASP:N	1:B:468:ASP:OD2	2.33	0.61
1:A:303:LEU:HD12	1:A:323:TYR:CA	2.31	0.61
1:C:135:ALA:O	1:C:136:ILE:HG13	2.01	0.61
1:D:533:LEU:HD12	1:D:536:LYS:H	1.66	0.61
1:D:779:ILE:CG1	1:D:871:LEU:HD21	2.31	0.61
1:A:276:LEU:CD2	1:A:341:ILE:HD13	2.30	0.61
1:B:85:MET:HE3	1:B:86:ASP:N	2.15	0.61
1:D:433:THR:O	1:D:462:MET:HE2	2.00	0.61
1:A:132:PRO:HB3	1:A:194:GLU:OE2	2.01	0.61
1:A:153:ASN:ND2	1:A:158:ASN:HB3	2.16	0.61
1:B:621:ASP:HB3	3:H:114:DA:H5''	1.83	0.61
1:C:78:ILE:HD11	1:C:80:LEU:HD23	1.82	0.61
1:C:195:LYS:HZ3	1:C:195:LYS:HB2	1.64	0.61
1:C:542:LEU:O	1:C:546:GLN:HG3	2.01	0.61
1:C:720:TYR:CE1	1:C:724:LYS:HD2	2.36	0.61
1:D:156:TYR:CD2	1:D:156:TYR:N	2.65	0.61
1:D:833:LEU:HB2	1:D:848:TRP:HH2	1.65	0.61
1:D:403:ARG:HH22	1:D:889:LEU:HD21	1.64	0.60
1:D:508:LEU:HD13	1:D:509:SER:N	2.15	0.60
1:B:504:HIS:O	1:B:506:PRO:HD3	2.01	0.60
1:C:642:ARG:HE	1:C:646:HIS:HD2	1.39	0.60
1:C:642:ARG:HH11	1:C:646:HIS:HB3	1.65	0.60
1:A:836:ARG:HG3	1:A:867:ASP:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TRP:CD2	1:B:566:LEU:HD13	2.36	0.60
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.82	0.60
3:H:110:DA:H2''	3:H:111:DT:H5'	1.83	0.60
1:C:454:TYR:CD2	1:C:462:MET:HE3	2.35	0.60
1:C:530:ILE:HD11	1:C:541:MET:HE1	1.81	0.60
1:D:412:LEU:HD21	1:D:683:MET:HE2	1.83	0.60
2:G:10:DA:H2''	2:G:11:DC:C5'	2.31	0.60
2:G:16:DG:H2''	2:G:17:DC:C5'	2.32	0.60
1:A:38:PHE:CD2	1:A:59:ARG:HA	2.36	0.60
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.16	0.60
1:A:772:ARG:HD2	1:A:868:TYR:CD2	2.36	0.60
1:B:270:VAL:C	1:B:271:LEU:HD12	2.26	0.60
1:C:203:ASN:O	1:C:207:GLN:HG2	2.01	0.60
1:D:216:TRP:HB2	1:D:290:LEU:HD12	1.83	0.60
1:D:402:ASN:CG	1:D:403:ARG:H	2.09	0.60
1:D:833:LEU:HB2	1:D:848:TRP:CH2	2.36	0.60
3:F:104:DG:C3'	3:F:105:DC:H5''	2.31	0.60
1:B:629:ALA:HA	1:B:632:ILE:HG12	1.82	0.60
1:D:151:LEU:HD13	1:D:151:LEU:C	2.27	0.60
1:D:191:PHE:HD1	1:D:197:LEU:HD23	1.65	0.60
1:D:191:PHE:CD1	1:D:197:LEU:HD23	2.35	0.60
1:A:725:LEU:HD11	1:A:750:ARG:HB2	1.82	0.60
1:B:85:MET:HE3	1:B:86:ASP:H	1.67	0.60
1:B:126:PRO:HG3	1:B:221:PHE:HD1	1.66	0.60
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.67	0.60
1:C:151:LEU:HD21	1:C:154:SER:HB3	1.83	0.60
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.83	0.60
1:A:783:SER:HA	3:F:111:DT:OP1	2.01	0.60
1:C:726:LYS:CE	1:C:728:MET:HE3	2.32	0.60
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.67	0.60
2:K:10:DA:H2''	2:K:11:DC:C5'	2.31	0.60
1:B:288:TYR:CD1	1:B:293:ILE:HD11	2.37	0.60
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.84	0.60
1:C:327:ALA:O	1:C:330:ARG:HB2	2.01	0.60
1:C:822:PRO:HD2	1:C:855:THR:OG1	2.01	0.60
1:A:137:THR:HB	1:A:328:VAL:HG21	1.83	0.59
1:A:194:GLU:OE1	1:A:229:ARG:NH1	2.34	0.59
1:A:485:HIS:C	1:A:487:GLY:N	2.59	0.59
1:A:813:ARG:HB2	1:A:813:ARG:HH11	1.67	0.59
1:C:37:LEU:C	1:C:38:PHE:CD1	2.80	0.59
1:D:231:LYS:O	1:D:235:GLY:HA2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG22	1:A:857:LEU:HG	1.83	0.59
1:B:505:ASN:ND2	1:B:507:ASN:ND2	2.46	0.59
1:D:194:GLU:O	1:D:198:LEU:HB2	2.02	0.59
1:A:482:ARG:HE	1:A:556:GLN:NE2	2.00	0.59
1:B:102:LYS:HD2	1:B:103:TYR:N	2.18	0.59
1:B:706:LYS:HD2	3:H:113:DC:H1'	1.84	0.59
1:B:777:ILE:HD11	1:B:853:GLU:CG	2.31	0.59
1:C:302:LYS:HD3	1:C:303:LEU:N	2.17	0.59
1:D:159:VAL:HG11	1:D:317:HIS:CG	2.37	0.59
1:D:835:LEU:CD2	1:D:846:ILE:HG23	2.33	0.59
1:A:132:PRO:HA	1:A:229:ARG:NH1	2.17	0.59
1:A:514:LEU:HD13	1:A:529:LYS:HZ3	1.68	0.59
1:D:503:LEU:HD23	1:D:503:LEU:O	2.03	0.59
1:B:504:HIS:C	1:B:506:PRO:HD3	2.28	0.59
1:C:685:ARG:HD2	1:C:685:ARG:C	2.28	0.59
1:D:68:ALA:O	1:D:71:TRP:HB3	2.02	0.59
1:D:136:ILE:HG23	1:D:149:PHE:HB2	1.83	0.59
2:I:10:DA:H2''	2:I:11:DC:C5'	2.32	0.59
1:A:839:ASN:HB2	1:A:840:PRO:CD	2.22	0.59
1:B:642:ARG:H	1:B:646:HIS:HD2	1.50	0.59
1:D:171:GLN:HE22	1:D:303:LEU:CD1	2.15	0.59
1:A:279:LYS:HD3	1:A:359:PHE:HD1	1.68	0.59
1:A:807:GLY:HA2	1:A:845:CYS:O	2.03	0.59
1:D:286:PRO:HB3	1:D:782:VAL:HG11	1.83	0.59
1:D:305:TYR:OH	1:D:309:ILE:HA	2.03	0.59
1:D:482:ARG:C	1:D:484:GLU:H	2.11	0.59
1:D:542:LEU:HD11	1:D:546:GLN:HE21	1.67	0.59
1:A:290:LEU:O	1:A:294:SER:HB2	2.03	0.59
1:A:811:TYR:CZ	1:A:815:ILE:HD13	2.38	0.59
1:D:598:GLU:HG3	1:D:617:VAL:HG21	1.83	0.59
1:D:777:ILE:HG23	1:D:831:TYR:CE1	2.37	0.59
1:A:708:TYR:C	1:A:708:TYR:CD2	2.81	0.59
1:C:170:LEU:HA	1:C:177:GLU:HG2	1.85	0.59
1:C:277:TYR:O	1:C:281:SER:HB3	2.03	0.59
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.84	0.59
1:D:132:PRO:HA	1:D:229:ARG:NH2	2.18	0.59
1:D:335:ASP:O	1:D:339:GLN:N	2.32	0.59
1:A:298:LEU:HD12	1:A:298:LEU:N	2.17	0.58
1:B:471:VAL:HG11	1:B:570:LEU:HD11	1.85	0.58
1:D:77:ASP:O	1:D:78:ILE:HD13	2.03	0.58
1:A:40:HIS:CD2	1:A:57:CYS:SG	2.95	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:HA	1:B:347:MET:HE3	1.84	0.58
1:B:505:ASN:HD22	1:B:507:ASN:ND2	2.01	0.58
1:C:274:ILE:HG23	1:C:275:ASP:N	2.17	0.58
1:D:770:GLU:O	1:D:774:LEU:HG	2.03	0.58
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.38	0.58
1:D:285:GLN:HE21	1:D:285:GLN:H	1.52	0.58
1:D:594:LEU:HD11	1:D:625:ILE:HG22	1.86	0.58
1:D:777:ILE:HG23	1:D:831:TYR:HE1	1.68	0.58
1:D:779:ILE:HG13	1:D:871:LEU:HD21	1.84	0.58
1:B:425:ILE:HG23	1:B:463:TYR:CE2	2.39	0.58
1:C:42:PRO:HG2	1:C:45:GLN:HG3	1.84	0.58
1:C:181:GLU:H	1:C:181:GLU:CD	2.11	0.58
1:D:381:PRO:O	1:D:576:ARG:HD2	2.03	0.58
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.85	0.58
1:D:848:TRP:CG	1:D:854:ILE:HB	2.38	0.58
3:J:111:DT:H2"	3:J:112:DT:H5"	1.85	0.58
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.38	0.58
1:A:120:PRO:HG2	1:A:156:TYR:CE1	2.39	0.58
1:A:364:THR:O	1:A:368:ILE:HG13	2.03	0.58
1:A:494:ARG:NH2	1:A:521:ASP:HB3	2.18	0.58
1:A:743:LYS:O	1:A:746:LYS:HB3	2.04	0.58
1:B:83:LEU:H	1:B:83:LEU:CD1	2.14	0.58
1:B:204:PHE:CE1	1:B:208:LYS:HD2	2.37	0.58
1:B:369:ILE:HG22	1:B:373:LEU:CD1	2.32	0.58
1:B:664:ASP:OD2	1:B:668:ARG:NH1	2.36	0.58
1:C:154:SER:C	1:C:156:TYR:N	2.61	0.58
1:C:825:VAL:HB	1:C:828:GLU:CD	2.28	0.58
1:D:197:LEU:O	1:D:197:LEU:HD22	2.04	0.58
1:D:397:LYS:O	1:D:399:PRO:HD3	2.02	0.58
1:A:467:ARG:HG3	1:A:467:ARG:NH1	2.18	0.58
1:B:739:LYS:HE2	1:B:742:GLN:HE22	1.66	0.58
1:C:788:ILE:HG13	1:C:826:GLU:OE1	2.04	0.58
1:D:82:ALA:H	1:D:382:GLN:HE21	1.50	0.58
1:D:786:ASN:HB2	3:L:110:DA:OP1	2.04	0.58
1:A:685:ARG:NH2	1:A:717:GLY:H	2.01	0.58
1:A:779:ILE:O	1:A:779:ILE:HG13	2.03	0.58
1:B:217:ASN:OD1	1:B:274:ILE:CD1	2.51	0.58
1:C:137:THR:HG21	1:C:325:ILE:HA	1.85	0.58
1:D:9:GLU:HG3	1:D:267:GLY:H	1.69	0.58
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.38	0.58
1:A:236:GLU:CG	1:A:240:LYS:HE2	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:DC:H2"	3:H:103:DG:OP2	2.04	0.58
1:B:317:HIS:O	1:B:320:TYR:HB3	2.04	0.58
1:C:831:TYR:CD2	1:C:850:SER:HA	2.38	0.57
1:A:42:PRO:HG2	1:A:45:GLN:HB2	1.86	0.57
1:A:523:SER:O	1:A:527:LYS:HB3	2.04	0.57
1:B:16:PHE:HB3	1:B:245:HIS:CE1	2.40	0.57
1:D:132:PRO:HA	1:D:229:ARG:HH21	1.68	0.57
1:D:305:TYR:CE2	1:D:312:LEU:HD13	2.39	0.57
1:A:708:TYR:CE2	1:A:728:MET:CG	2.85	0.57
1:B:117:VAL:CG2	1:B:133:ILE:HG12	2.34	0.57
1:B:855:THR:HG21	1:B:857:LEU:HD12	1.86	0.57
1:D:229:ARG:HH11	1:D:233:ILE:HD11	1.68	0.57
2:I:4:CTG:H5"	2:I:4:CTG:O6	2.03	0.57
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.16	0.57
1:A:405:LYS:O	1:A:690:GLY:HA2	2.04	0.57
1:A:410:PHE:HB2	1:A:683:MET:HE2	1.85	0.57
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.34	0.57
1:C:193:ASN:HD22	1:C:195:LYS:HZ1	1.51	0.57
1:D:313:ARG:HG3	1:D:317:HIS:CD2	2.40	0.57
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.39	0.57
1:C:183:ILE:HD12	1:C:186:ILE:CD1	2.33	0.57
1:D:150:ASP:HB3	1:D:188:TYR:CE1	2.36	0.57
1:D:347:MET:HG2	1:D:358:VAL:HG13	1.87	0.57
1:D:518:TYR:CD1	1:D:518:TYR:N	2.73	0.57
1:D:810:THR:HG22	1:D:846:ILE:HG22	1.85	0.57
1:A:109:ARG:NH1	1:A:140:ASP:OD2	2.37	0.57
1:A:839:ASN:CB	1:A:840:PRO:HD2	2.22	0.57
1:B:273:TYR:HA	1:B:276:LEU:HB2	1.87	0.57
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.40	0.57
1:C:231:LYS:HD2	1:C:231:LYS:O	2.05	0.57
1:D:15:ILE:HG23	1:D:65:MET:HE1	1.87	0.57
1:D:290:LEU:HD23	1:D:290:LEU:O	2.04	0.57
1:D:503:LEU:HG	1:D:535:ALA:HB2	1.85	0.57
1:A:602:ASN:ND2	1:A:616:PHE:HB2	2.20	0.57
1:B:210:PRO:HG2	1:B:213:LEU:HD13	1.86	0.57
1:B:835:LEU:HD21	1:B:862:VAL:HG13	1.85	0.57
1:C:465:LYS:NZ	1:C:675:ASN:ND2	2.53	0.57
1:D:214:THR:O	1:D:218:VAL:HG21	2.04	0.57
1:D:295:GLU:OE1	1:D:302:LYS:HG3	2.05	0.57
1:D:365:TRP:CE2	1:D:566:LEU:HD13	2.40	0.57
1:B:342:ASN:HB2	4:B:923:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ARG:H	1:B:646:HIS:CD2	2.23	0.57
1:C:231:LYS:C	1:C:231:LYS:HE2	2.29	0.57
1:C:811:TYR:HA	1:C:846:ILE:HD11	1.86	0.57
1:D:249:ARG:O	1:D:264:THR:HG22	2.05	0.57
1:D:285:GLN:H	1:D:285:GLN:NE2	2.02	0.57
1:A:395:PHE:HA	4:A:942:HOH:O	2.03	0.57
1:C:124:PRO:HB2	1:C:225:TYR:HE2	1.68	0.57
1:D:214:THR:HG21	1:D:273:TYR:HD2	1.69	0.57
1:D:405:LYS:O	1:D:690:GLY:HA2	2.05	0.57
1:D:534:SER:O	1:D:538:LEU:HD13	2.05	0.57
1:A:37:LEU:HD11	1:A:72:ILE:HD11	1.86	0.57
1:A:66:ARG:O	1:A:70:GLN:HB2	2.04	0.57
1:A:129:ALA:HA	1:A:225:TYR:CZ	2.39	0.57
1:A:654:PHE:HE1	1:A:659:MET:HG3	1.69	0.57
1:A:862:VAL:O	1:A:865:TRP:N	2.36	0.57
1:C:139:TYR:C	1:C:139:TYR:CD1	2.83	0.57
3:F:109:DC:H1'	3:F:110:DA:H5''	1.87	0.57
3:L:101:DG:H2''	3:L:102:DC:C6	2.40	0.57
1:A:824:VAL:HG11	1:A:830:VAL:HG12	1.87	0.56
1:B:117:VAL:HG13	1:B:132:PRO:O	2.05	0.56
1:B:347:MET:CE	1:B:350:TYR:HD2	2.18	0.56
1:B:858:ILE:O	1:B:862:VAL:HG23	2.04	0.56
1:D:101:ILE:HG22	1:D:102:LYS:N	2.20	0.56
1:D:270:VAL:O	1:D:271:LEU:HD23	2.05	0.56
1:B:505:ASN:HB3	1:B:535:ALA:CB	2.35	0.56
1:B:818:ASN:O	1:B:819:ILE:C	2.48	0.56
1:D:229:ARG:HH11	1:D:229:ARG:HG2	1.69	0.56
1:D:546:GLN:HA	1:D:549:GLU:HB3	1.87	0.56
1:A:411:ASP:OD1	1:A:686:GLU:HG3	2.06	0.56
1:A:514:LEU:CD2	1:A:529:LYS:HE2	2.36	0.56
1:A:654:PHE:CE1	1:A:659:MET:HG3	2.41	0.56
1:A:876:PHE:O	1:A:879:PRO:HG2	2.04	0.56
1:B:376:GLN:NE2	1:B:378:LYS:NZ	2.52	0.56
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.85	0.56
1:B:878:LYS:HD3	1:B:878:LYS:C	2.31	0.56
1:C:149:PHE:O	1:C:197:LEU:HD11	2.05	0.56
1:D:305:TYR:HE2	1:D:312:LEU:HD13	1.70	0.56
1:D:376:GLN:HB2	1:D:378:LYS:HG2	1.85	0.56
1:D:573:VAL:C	1:D:575:PHE:H	2.13	0.56
1:D:575:PHE:CE2	1:D:577:TYR:HB2	2.39	0.56
2:G:15:DC:H6	2:G:15:DC:H5'	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:110:DA:H1'	3:J:111:DT:H5''	1.87	0.56
1:B:159:VAL:HG11	1:B:313:ARG:O	2.05	0.56
1:C:451:SER:OG	1:C:453:VAL:HG22	2.05	0.56
1:D:89:LYS:O	1:D:93:LEU:HD13	2.05	0.56
1:D:202:LEU:HD21	1:D:241:ARG:CD	2.18	0.56
1:D:810:THR:CG2	1:D:846:ILE:HG22	2.36	0.56
3:F:110:DA:H1'	3:F:111:DT:H5''	1.87	0.56
1:B:821:ALA:HB1	1:B:822:PRO:HD2	1.87	0.56
1:C:139:TYR:CE2	1:C:332:LEU:HD21	2.41	0.56
1:C:731:GLU:HA	1:C:734:LYS:HG3	1.88	0.56
1:D:293:ILE:HD12	1:D:293:ILE:C	2.30	0.56
1:D:878:LYS:O	1:D:881:GLU:HB2	2.06	0.56
2:G:6:DA:H2''	2:G:7:DA:H5'	1.87	0.56
1:A:481:GLN:O	1:A:484:GLU:HB3	2.05	0.56
1:A:509:SER:H	1:A:534:SER:HB3	1.71	0.56
1:A:509:SER:N	1:A:534:SER:HB3	2.19	0.56
1:B:25:ARG:HG2	1:B:25:ARG:HH11	1.70	0.56
1:B:166:ILE:HD12	1:B:166:ILE:N	2.18	0.56
1:B:738:PRO:HB2	1:B:741:VAL:HB	1.88	0.56
1:C:9:GLU:OE2	1:C:266:PHE:HA	2.05	0.56
1:C:316:ASN:OD1	1:C:318:GLN:HB3	2.06	0.56
1:C:461:MET:SD	1:C:581:ARG:HD2	2.45	0.56
1:D:213:LEU:HD22	1:D:218:VAL:HG11	1.87	0.56
1:D:264:THR:HG23	1:D:264:THR:O	2.06	0.56
1:D:552:GLY:O	1:D:556:GLN:HB3	2.06	0.56
1:A:399:PRO:HG2	1:A:704:GLY:HA2	1.87	0.56
1:B:644:THR:HG23	1:B:645:ASN:N	2.21	0.56
1:C:189:MET:O	1:C:191:PHE:CE1	2.59	0.56
1:C:380:ILE:HD12	1:C:576:ARG:CZ	2.35	0.56
1:C:475:ILE:HG23	1:C:476:THR:N	2.20	0.56
1:C:506:PRO:HB3	1:C:535:ALA:HB2	1.87	0.56
1:D:180:SER:C	1:D:182:ILE:H	2.12	0.56
1:D:365:TRP:HA	1:D:368:ILE:HD12	1.87	0.56
3:J:105:DC:H2'	3:J:106:DT:C7	2.35	0.56
1:A:4:PHE:N	1:A:4:PHE:CD1	2.74	0.56
1:A:246:ARG:HG2	1:A:246:ARG:NH1	2.20	0.56
1:C:514:LEU:HB3	1:C:541:MET:HE3	1.87	0.56
1:C:592:MET:O	1:C:593:ALA:C	2.49	0.56
1:D:347:MET:HE1	1:D:562:LEU:HB2	1.88	0.56
1:D:830:VAL:HA	1:D:850:SER:HB3	1.88	0.56
1:A:653:LYS:HD3	1:A:657:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:LYS:HZ2	1:C:675:ASN:ND2	2.03	0.56
1:C:642:ARG:HE	1:C:646:HIS:CG	2.19	0.56
1:C:720:TYR:CZ	1:C:724:LYS:HD2	2.40	0.56
1:D:15:ILE:O	1:D:15:ILE:HG13	2.04	0.56
1:D:132:PRO:HA	1:D:229:ARG:CZ	2.35	0.56
1:D:154:SER:HB2	1:D:313:ARG:NH1	2.20	0.56
1:D:419:ILE:HD13	1:D:589:PHE:HD1	1.69	0.56
1:D:453:VAL:HG23	1:D:454:TYR:CD1	2.40	0.56
1:D:777:ILE:O	1:D:777:ILE:CG2	2.53	0.56
3:J:105:DC:H5'	3:J:105:DC:H6	1.71	0.56
1:A:4:PHE:O	1:A:19:TYR:HB2	2.05	0.56
1:C:154:SER:O	1:C:156:TYR:N	2.39	0.56
1:A:501:GLU:HA	1:A:504:HIS:CE1	2.41	0.55
1:A:880:LEU:O	1:A:883:PHE:HB2	2.05	0.55
1:D:347:MET:HE2	1:D:558:ASN:ND2	2.21	0.55
1:D:455:SER:HA	1:D:675:ASN:O	2.06	0.55
1:D:554:THR:O	1:D:558:ASN:HB2	2.06	0.55
3:J:105:DC:C5'	3:J:105:DC:H6	2.19	0.55
1:A:19:TYR:HE1	1:A:29:ARG:HG2	1.71	0.55
1:A:686:GLU:O	1:A:716:GLU:N	2.33	0.55
1:C:214:THR:HG21	1:C:341:ILE:HD11	1.88	0.55
1:D:48:LYS:O	1:D:377:ASN:HB3	2.06	0.55
1:D:131:HIS:O	1:D:229:ARG:NE	2.39	0.55
3:H:105:DC:H2'	3:H:106:DT:H71	1.86	0.55
1:A:489:MET:SD	1:A:553:MET:HG2	2.46	0.55
1:B:85:MET:CE	1:B:87:ASP:H	2.09	0.55
1:B:516:VAL:CG1	1:B:544:ARG:HH11	2.18	0.55
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.42	0.55
1:D:109:ARG:HH21	1:D:208:LYS:CB	2.19	0.55
1:D:442:TYR:HB3	1:D:592:MET:CE	2.34	0.55
1:D:513:PRO:HA	1:D:541:MET:CE	2.36	0.55
1:D:516:VAL:HG12	1:D:517:ASP:N	2.21	0.55
1:A:113:PHE:CE1	1:A:218:VAL:HG21	2.42	0.55
1:A:211:VAL:HG12	1:A:212:ILE:HG12	1.89	0.55
1:A:362:ILE:HD11	1:A:572:ASN:HD22	1.70	0.55
1:A:365:TRP:O	1:A:366:ASP:C	2.50	0.55
1:B:113:PHE:HB2	1:B:137:THR:O	2.07	0.55
1:B:668:ARG:HH11	1:B:668:ARG:CG	2.14	0.55
1:C:499:ILE:CG2	1:C:542:LEU:HB2	2.37	0.55
1:D:197:LEU:HD13	1:D:197:LEU:C	2.31	0.55
1:D:458:PRO:C	1:D:460:GLY:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ILE:HG12	1:A:667:PHE:CE2	2.41	0.55
1:A:781:SER:O	1:A:831:TYR:HA	2.06	0.55
1:B:129:ALA:HB1	1:B:229:ARG:CD	2.36	0.55
1:B:145:ARG:HG3	1:B:185:LYS:O	2.07	0.55
1:B:796:PHE:CD1	1:B:813:ARG:NH1	2.74	0.55
1:C:528:GLU:HA	1:C:528:GLU:OE2	2.07	0.55
1:C:791:TYR:HD2	1:C:801:CYS:HA	1.68	0.55
1:D:741:VAL:HG12	1:D:745:LEU:HG	1.88	0.55
1:D:824:VAL:HG23	1:D:830:VAL:HG11	1.87	0.55
1:A:604:TYR:O	1:A:608:VAL:HG22	2.07	0.55
1:A:759:SER:O	1:A:760:LEU:C	2.48	0.55
1:B:115:ILE:HD13	1:B:115:ILE:H	1.71	0.55
2:G:10:DA:H2''	2:G:11:DC:H5''	1.89	0.55
1:A:414:SER:O	1:A:417:PRO:HD2	2.07	0.55
1:B:3:GLU:HG2	1:B:21:ASP:HA	1.89	0.55
1:B:20:ILE:HG22	1:B:24:GLY:HA2	1.87	0.55
1:B:147:TYR:N	1:B:147:TYR:CD1	2.75	0.55
1:B:772:ARG:NH2	1:B:868:TYR:HB2	2.21	0.55
1:C:251:LYS:HB3	1:C:262:ILE:HG13	1.87	0.55
1:C:326:ILE:O	1:C:327:ALA:C	2.49	0.55
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.36	0.55
1:A:420:ILE:HG12	1:A:586:ILE:HD11	1.87	0.55
1:A:846:ILE:HD12	1:A:847:ALA:O	2.07	0.55
1:B:792:ASP:HA	1:B:809:LEU:HD21	1.87	0.55
1:B:878:LYS:HD3	1:B:878:LYS:O	2.06	0.55
1:C:202:LEU:HD23	1:C:241:ARG:HH21	1.72	0.55
1:D:52:ILE:CG2	1:D:381:PRO:HD3	2.37	0.55
1:D:159:VAL:HG21	1:D:317:HIS:CD2	2.42	0.55
1:D:814:ALA:HB3	1:D:841:PHE:CD1	2.41	0.55
2:E:16:DG:N2	3:F:103:DG:N2	2.54	0.55
1:A:310:SER:C	1:A:311:LYS:HD3	2.32	0.55
1:A:659:MET:O	1:A:660:GLU:C	2.50	0.55
1:B:376:GLN:NE2	1:B:378:LYS:HZ2	2.05	0.55
1:C:41:CYS:CB	1:C:58:THR:HG22	2.25	0.55
1:C:81:GLU:HG2	1:C:83:LEU:CD2	2.36	0.55
1:D:395:PHE:HB3	1:D:594:LEU:HD23	1.89	0.55
2:G:15:DC:H2''	2:G:16:DG:O5'	2.06	0.55
1:A:782:VAL:HG22	1:A:831:TYR:HD1	1.71	0.55
1:B:182:ILE:O	1:B:186:ILE:HG13	2.07	0.55
1:B:433:THR:O	1:B:462:MET:HE2	2.06	0.55
1:A:517:ASP:OD1	1:A:519:ARG:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:HB3	1:B:147:TYR:CE1	2.41	0.54
1:B:488:TYR:C	1:B:490:LEU:H	2.16	0.54
1:C:111:ALA:HB3	1:C:210:PRO:HB3	1.89	0.54
1:C:195:LYS:HZ3	1:C:195:LYS:CB	2.21	0.54
1:C:392:PRO:HG2	1:C:584:THR:HG23	1.89	0.54
2:I:12:DA:H2''	2:I:13:DG:H5'	1.89	0.54
1:A:592:MET:HE1	1:A:674:MET:CG	2.37	0.54
1:A:702:TRP:CD1	1:A:708:TYR:HB3	2.42	0.54
1:D:216:TRP:CH2	1:D:293:ILE:HG12	2.41	0.54
1:D:512:GLU:CB	1:D:513:PRO:CA	2.85	0.54
1:D:530:ILE:O	1:D:532:LYS:N	2.40	0.54
3:F:107:DG:H2''	3:F:108:DT:OP2	2.06	0.54
1:A:4:PHE:CE2	1:A:103:TYR:HB2	2.42	0.54
1:B:116:GLU:N	1:B:135:ALA:O	2.39	0.54
1:B:621:ASP:HB3	3:H:114:DA:C5'	2.36	0.54
1:B:898:PHE:HD1	1:B:898:PHE:H	1.55	0.54
1:D:450:PRO:HB2	1:D:456:CYS:SG	2.48	0.54
1:D:514:LEU:HD11	1:D:532:LYS:CB	2.37	0.54
1:A:41:CYS:HB3	1:A:58:THR:HG22	1.89	0.54
1:A:782:VAL:HG12	1:A:783:SER:N	2.22	0.54
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.17	0.54
1:C:147:TYR:HB3	1:C:149:PHE:CE1	2.42	0.54
1:A:798:GLY:N	1:A:801:CYS:SG	2.80	0.54
1:B:421:ARG:HG2	1:B:421:ARG:NH1	2.23	0.54
1:C:138:HIS:C	1:C:138:HIS:CD2	2.85	0.54
1:C:143:ASP:O	1:C:144:ASP:HB3	2.07	0.54
1:C:738:PRO:HG2	1:C:741:VAL:CG2	2.37	0.54
1:D:514:LEU:N	1:D:514:LEU:HD12	2.22	0.54
1:D:750:ARG:NH1	1:D:754:GLN:NE2	2.55	0.54
1:A:279:LYS:HE3	1:A:280:PHE:CE1	2.42	0.54
1:A:395:PHE:HB2	1:A:591:GLN:OE1	2.08	0.54
1:A:835:LEU:HD21	1:A:846:ILE:HG21	1.88	0.54
1:B:395:PHE:HB2	1:B:591:GLN:NE2	2.11	0.54
1:B:836:ARG:NH2	1:B:864:HIS:O	2.41	0.54
1:C:375:GLU:HA	1:C:375:GLU:OE2	2.08	0.54
1:D:848:TRP:HB2	1:D:849:PRO:HD2	1.88	0.54
2:G:12:DA:H2''	2:G:13:DG:O5'	2.08	0.54
1:A:362:ILE:CD1	1:A:569:ALA:HA	2.37	0.54
1:A:373:LEU:HD11	1:A:470:VAL:HG11	1.90	0.54
1:A:782:VAL:HG22	1:A:831:TYR:CD1	2.43	0.54
1:B:361:PRO:HB3	1:B:565:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:C	1:B:376:GLN:H	2.16	0.54
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.23	0.54
1:D:13:ASP:HB3	1:D:64:ASN:HB2	1.88	0.54
1:D:600:LYS:HE3	1:D:669:GLU:OE2	2.08	0.54
1:A:835:LEU:HD11	1:A:846:ILE:CG2	2.29	0.54
1:B:389:GLN:CD	1:B:390:PRO:HD2	2.32	0.54
1:B:609:CYS:HA	1:B:635:LYS:HE3	1.90	0.54
1:C:143:ASP:OD2	1:C:208:LYS:NZ	2.37	0.54
1:C:215:GLY:HA3	1:C:218:VAL:CG2	2.37	0.54
1:D:312:LEU:HG	1:D:320:TYR:HB2	1.90	0.54
1:A:408:MET:HG2	1:A:688:ILE:HG12	1.90	0.54
1:A:840:PRO:C	1:A:842:GLY:N	2.65	0.54
1:B:353:ILE:HG13	1:B:354:GLN:O	2.07	0.54
1:C:135:ALA:O	1:C:136:ILE:CG1	2.56	0.54
1:C:836:ARG:HH11	1:C:836:ARG:HG3	1.73	0.54
1:D:856:ASP:HA	1:D:859:LYS:CB	2.38	0.54
1:A:897:LEU:H	1:A:897:LEU:CD1	2.16	0.54
1:B:118:THR:OG1	1:B:313:ARG:HD2	2.07	0.54
1:B:629:ALA:CA	1:B:632:ILE:HG12	2.38	0.54
1:C:373:LEU:HD22	1:C:378:LYS:HD2	1.88	0.54
1:C:453:VAL:HG23	1:C:454:TYR:N	2.23	0.54
1:D:286:PRO:O	1:D:829:LYS:HD3	2.08	0.54
1:D:488:TYR:HD1	1:D:519:ARG:HH21	1.56	0.54
1:B:112:ASN:O	1:B:113:PHE:HB3	2.08	0.53
1:B:120:PRO:HG2	1:B:156:TYR:CE2	2.43	0.53
1:B:376:GLN:HE21	1:B:378:LYS:HZ2	1.56	0.53
1:C:171:GLN:C	1:C:173:GLN:H	2.16	0.53
1:D:140:ASP:CB	1:D:143:ASP:HB3	2.35	0.53
1:D:368:ILE:CD1	1:D:562:LEU:HD11	2.39	0.53
1:D:697:GLY:HA3	1:D:753:LEU:O	2.07	0.53
1:A:108:ILE:HG23	1:A:211:VAL:HG11	1.89	0.53
1:A:668:ARG:O	1:A:672:GLU:HG3	2.09	0.53
1:B:130:LYS:HB2	1:B:130:LYS:HZ2	1.73	0.53
1:B:273:TYR:O	1:B:277:TYR:N	2.39	0.53
1:C:215:GLY:HA3	1:C:218:VAL:HG21	1.90	0.53
1:D:156:TYR:N	1:D:156:TYR:HD2	2.05	0.53
1:D:285:GLN:NE2	1:D:285:GLN:N	2.56	0.53
1:D:300:VAL:HG12	1:D:301:GLY:N	2.23	0.53
1:D:807:GLY:HA2	1:D:845:CYS:O	2.07	0.53
1:B:177:GLU:HG2	1:B:303:LEU:HD11	1.90	0.53
1:C:109:ARG:HG2	1:C:210:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HD13	1:D:26:GLU:HA	1.90	0.53
1:D:883:PHE:CD2	1:D:883:PHE:N	2.76	0.53
3:H:106:DT:H2''	3:H:107:DG:O5'	2.07	0.53
3:L:101:DG:H2''	3:L:102:DC:C5	2.42	0.53
1:B:216:TRP:CH2	1:B:293:ILE:HG21	2.43	0.53
1:B:516:VAL:HG22	1:B:517:ASP:N	2.22	0.53
1:B:831:TYR:CE2	1:B:850:SER:HA	2.43	0.53
1:C:71:TRP:O	1:C:75:MET:HG2	2.07	0.53
2:G:14:DC:H2''	2:G:15:DC:C5'	2.38	0.53
1:B:147:TYR:HD1	1:B:147:TYR:H	1.56	0.53
1:C:35:PRO:HD3	1:C:65:MET:HG2	1.91	0.53
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.44	0.53
1:C:163:SER:OG	1:C:166:ILE:HG13	2.09	0.53
1:C:362:ILE:HD12	1:C:575:PHE:HB2	1.89	0.53
2:G:3:DT:H2''	2:G:4:CTG:OP2	2.08	0.53
1:A:313:ARG:O	1:A:317:HIS:HB2	2.09	0.53
1:A:776:TYR:CZ	1:A:777:ILE:HG13	2.43	0.53
1:C:163:SER:CB	1:C:166:ILE:HD12	2.39	0.53
1:C:347:MET:HE1	1:C:562:LEU:HD13	1.91	0.53
1:D:271:LEU:HB3	1:D:276:LEU:HD11	1.91	0.53
1:D:617:VAL:HG23	1:D:617:VAL:O	2.09	0.53
1:D:825:VAL:HB	1:D:828:GLU:CG	2.38	0.53
1:D:839:ASN:HD22	1:D:839:ASN:N	2.04	0.53
1:A:509:SER:H	1:A:534:SER:CB	2.22	0.53
1:A:693:LEU:HD12	1:A:694:GLY:N	2.23	0.53
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.08	0.53
1:B:456:CYS:SG	1:B:462:MET:HG2	2.49	0.53
1:B:597:ILE:HD13	1:B:667:PHE:CZ	2.44	0.53
1:B:825:VAL:HB	1:B:828:GLU:HG3	1.91	0.53
1:D:305:TYR:HE1	1:D:309:ILE:HG22	1.74	0.53
1:D:815:ILE:CG2	1:D:858:ILE:HG21	2.26	0.53
1:D:864:HIS:C	1:D:866:MET:N	2.67	0.53
1:D:864:HIS:O	1:D:866:MET:N	2.36	0.53
2:G:8:DT:C2'	2:G:9:DG:C8	2.92	0.53
1:A:48:LYS:HE3	1:A:377:ASN:OD1	2.09	0.53
1:D:668:ARG:HG3	1:D:679:HIS:CE1	2.43	0.53
1:A:153:ASN:HD22	1:A:158:ASN:HB3	1.73	0.53
1:A:840:PRO:O	1:A:842:GLY:N	2.41	0.53
1:C:148:VAL:C	1:C:149:PHE:CD1	2.87	0.53
1:C:833:LEU:HD13	1:C:866:MET:HE3	1.89	0.53
1:D:8:VAL:HG11	1:D:93:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:HIS:HB3	1:D:556:GLN:CB	2.39	0.53
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.90	0.53
1:A:362:ILE:HG12	1:A:572:ASN:HD22	1.74	0.53
1:A:706:LYS:CE	3:F:113:DC:O2	2.56	0.53
1:C:686:GLU:OE1	1:C:716:GLU:HG3	2.09	0.53
1:D:147:TYR:CE2	1:D:187:ILE:HD13	2.44	0.53
1:D:402:ASN:CG	1:D:403:ARG:N	2.66	0.53
1:D:546:GLN:O	1:D:550:VAL:HG23	2.09	0.53
1:D:738:PRO:HB2	1:D:778:SER:O	2.08	0.53
1:A:612:GLU:HG2	1:A:612:GLU:O	2.09	0.52
1:A:622:THR:HG22	1:A:623:ASP:N	2.24	0.52
1:A:789:ALA:O	1:A:791:TYR:N	2.42	0.52
1:B:186:ILE:O	1:B:187:ILE:HG13	2.09	0.52
1:C:85:MET:HE3	1:C:370:PHE:CD1	2.44	0.52
1:C:195:LYS:H	1:C:195:LYS:HZ2	1.50	0.52
1:C:645:ASN:OD1	1:C:719:ARG:NH1	2.40	0.52
1:D:416:TYR:HD2	1:D:586:ILE:CG2	2.22	0.52
1:A:422:GLN:HE21	1:A:680:LEU:H	1.54	0.52
1:A:516:VAL:HG21	1:A:522:PHE:CE2	2.44	0.52
1:A:625:ILE:HG13	1:A:625:ILE:O	2.08	0.52
1:B:159:VAL:HG22	1:B:313:ARG:HH22	1.75	0.52
1:B:747:GLU:HG2	1:B:763:TYR:CZ	2.44	0.52
1:C:119:SER:HA	1:C:131:HIS:CD2	2.43	0.52
1:C:204:PHE:HE1	1:C:208:LYS:HG3	1.74	0.52
1:C:855:THR:HG22	1:C:857:LEU:N	2.19	0.52
1:D:114:ASP:CB	1:D:328:VAL:HG13	2.39	0.52
1:A:708:TYR:C	1:A:708:TYR:HD2	2.18	0.52
1:A:855:THR:CG2	1:A:857:LEU:HG	2.39	0.52
1:B:11:ILE:HD12	1:B:16:PHE:CD1	2.44	0.52
1:B:51:ASP:C	1:B:51:ASP:OD1	2.51	0.52
1:B:117:VAL:HG22	1:B:132:PRO:O	2.10	0.52
1:B:162:TRP:HA	1:B:318:GLN:NE2	2.20	0.52
1:B:218:VAL:HG12	1:B:223:ILE:HD11	1.91	0.52
1:B:810:THR:HG23	1:B:813:ARG:HH21	1.74	0.52
1:B:887:ALA:HB1	1:B:889:LEU:HD12	1.91	0.52
1:C:493:GLN:HG3	1:C:549:GLU:OE2	2.10	0.52
1:D:543:PHE:O	1:D:547:ARG:HB3	2.10	0.52
1:A:471:VAL:HB	1:A:472:PRO:CD	2.38	0.52
1:A:727:ILE:HD13	1:A:749:ILE:HD12	1.90	0.52
1:A:804:HIS:HE2	3:F:110:DA:P	2.32	0.52
1:B:206:GLN:HE22	1:B:246:ARG:HH22	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:O	1:B:233:ILE:HD13	2.09	0.52
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.22	0.52
1:C:412:LEU:HD13	1:C:415:LEU:CD1	2.39	0.52
1:D:403:ARG:NH2	1:D:889:LEU:HD21	2.24	0.52
1:A:824:VAL:CG1	1:A:849:PRO:HG3	2.39	0.52
1:B:499:ILE:H	1:B:499:ILE:CD1	2.04	0.52
1:A:153:ASN:HB3	1:A:158:ASN:HD22	1.74	0.52
1:B:166:ILE:H	1:B:166:ILE:CD1	2.19	0.52
1:C:202:LEU:O	1:C:205:TRP:HB3	2.10	0.52
1:C:353:ILE:HD12	1:C:357:SER:HB3	1.91	0.52
1:D:170:LEU:CD2	1:D:177:GLU:HG2	2.40	0.52
1:D:191:PHE:HB2	1:D:197:LEU:HB2	1.92	0.52
1:D:514:LEU:H	1:D:541:MET:HE1	1.74	0.52
2:K:6:DA:H2''	2:K:7:DA:H5'	1.91	0.52
1:A:68:ALA:O	1:A:72:ILE:HG13	2.09	0.52
1:A:858:ILE:O	1:A:862:VAL:HG23	2.10	0.52
1:B:93:LEU:HD23	1:B:352:LYS:O	2.10	0.52
1:C:51:ASP:OD2	1:C:51:ASP:C	2.52	0.52
1:D:136:ILE:HD11	1:D:201:TYR:CZ	2.45	0.52
1:D:514:LEU:CD1	1:D:541:MET:HE1	2.40	0.52
1:D:725:LEU:HG	1:D:746:LYS:HZ2	1.75	0.52
1:D:874:LYS:HG3	1:D:875:THR:HG23	1.92	0.52
1:A:301:GLY:O	1:A:330:ARG:NE	2.33	0.52
1:A:347:MET:HA	1:A:347:MET:CE	2.38	0.52
1:B:474:GLU:OE2	1:B:477:LYS:HD2	2.10	0.52
1:B:594:LEU:HG	1:B:594:LEU:O	2.10	0.52
1:B:625:ILE:O	1:B:625:ILE:HG13	2.10	0.52
1:C:53:TYR:CE1	1:C:428:GLU:HA	2.45	0.52
1:C:188:TYR:C	1:C:189:MET:HG3	2.34	0.52
1:C:241:ARG:HA	1:C:246:ARG:HD3	1.91	0.52
1:C:534:SER:O	1:C:538:LEU:HG	2.09	0.52
1:C:793:VAL:HG12	1:C:793:VAL:O	2.10	0.52
1:A:75:MET:HE3	1:A:80:LEU:O	2.09	0.52
1:A:135:ALA:HA	1:A:149:PHE:O	2.08	0.52
1:B:422:GLN:HG3	1:B:678:GLN:O	2.10	0.52
1:B:808:ILE:HG22	1:B:812:ASN:ND2	2.20	0.52
1:C:169:LYS:O	1:C:175:GLY:HA3	2.09	0.52
1:C:214:THR:HB	1:C:271:LEU:O	2.10	0.52
1:D:113:PHE:HB2	1:D:137:THR:O	2.10	0.52
1:D:413:THR:O	1:D:414:SER:C	2.52	0.52
1:D:619:TYR:OH	1:D:706:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:O	1:A:106:THR:N	2.43	0.52
1:A:529:LYS:HZ3	1:A:529:LYS:HB3	1.75	0.52
1:A:806:ARG:HD3	1:A:843:ASP:OD2	2.09	0.52
1:B:489:MET:HE3	1:B:553:MET:SD	2.49	0.52
1:D:644:THR:O	1:D:648:VAL:HG23	2.09	0.52
1:A:740:ALA:HB2	1:A:778:SER:HB2	1.90	0.51
1:B:51:ASP:OD1	1:B:53:TYR:N	2.43	0.51
1:B:96:THR:HG22	1:B:97:TYR:CE2	2.45	0.51
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.44	0.51
1:B:752:MET:HE3	1:B:889:LEU:HD12	1.91	0.51
1:C:170:LEU:HA	1:C:177:GLU:CG	2.40	0.51
1:C:659:MET:O	1:C:660:GLU:C	2.53	0.51
1:C:752:MET:HG2	1:C:889:LEU:CD1	2.40	0.51
1:C:878:LYS:HB3	1:C:879:PRO:CD	2.40	0.51
1:D:813:ARG:O	1:D:815:ILE:N	2.38	0.51
3:J:105:DC:H2'	3:J:106:DT:C6	2.44	0.51
1:A:897:LEU:HD12	1:A:897:LEU:N	2.18	0.51
1:A:898:PHE:H	1:A:898:PHE:HD1	1.56	0.51
1:A:901:PHE:O	1:A:902:ASP:HB2	2.09	0.51
1:B:124:PRO:O	1:B:125:GLU:C	2.53	0.51
1:B:728:MET:HG3	3:H:113:DC:C5'	2.39	0.51
1:C:146:PHE:CD1	1:C:146:PHE:N	2.78	0.51
1:D:52:ILE:HG23	1:D:381:PRO:HD3	1.92	0.51
1:D:87:ASP:OD1	1:D:89:LYS:HG2	2.11	0.51
1:A:592:MET:HE1	1:A:674:MET:HG3	1.92	0.51
1:A:829:LYS:O	1:A:830:VAL:HG13	2.10	0.51
1:A:880:LEU:HD22	1:A:884:THR:HG23	1.92	0.51
1:C:482:ARG:HH12	1:C:556:GLN:NE2	2.03	0.51
1:C:482:ARG:HB2	1:C:559:ARG:HB3	1.93	0.51
1:D:17:GLU:HG2	1:D:18:ARG:N	2.24	0.51
1:D:171:GLN:HE22	1:D:303:LEU:HD13	1.75	0.51
1:A:153:ASN:HB3	1:A:158:ASN:ND2	2.25	0.51
1:A:607:GLU:C	1:A:609:CYS:H	2.19	0.51
1:B:71:TRP:HZ2	1:B:75:MET:HE3	1.74	0.51
1:B:116:GLU:HB3	1:B:135:ALA:HB3	1.93	0.51
1:B:253:ILE:HD12	1:B:254:GLU:N	2.25	0.51
1:C:347:MET:CE	1:C:562:LEU:HD13	2.41	0.51
1:D:263:ILE:HD12	1:D:263:ILE:N	2.26	0.51
1:D:508:LEU:HD23	1:D:534:SER:HB2	1.92	0.51
2:G:16:DG:C2'	2:G:17:DC:H5''	2.40	0.51
1:A:126:PRO:HA	1:A:225:TYR:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:CG1	1:A:572:ASN:ND2	2.71	0.51
1:A:499:ILE:HD13	1:A:541:MET:HG2	1.92	0.51
1:A:767:PHE:O	1:A:767:PHE:CD1	2.64	0.51
1:B:525:GLU:O	1:B:526:ILE:HG23	2.11	0.51
1:C:308:PRO:CG	1:C:311:LYS:HG2	2.41	0.51
1:D:178:VAL:HG22	1:D:326:ILE:HD11	1.92	0.51
1:D:290:LEU:HD23	1:D:290:LEU:C	2.35	0.51
1:D:434:PHE:CZ	1:D:460:GLY:HA2	2.46	0.51
1:D:645:ASN:OD1	1:D:719:ARG:NH1	2.44	0.51
1:D:813:ARG:HG3	1:D:814:ALA:N	2.24	0.51
1:A:685:ARG:NH2	1:A:717:GLY:N	2.59	0.51
1:A:785:ALA:C	1:A:786:ASN:HD22	2.19	0.51
1:B:197:LEU:HD23	1:B:197:LEU:C	2.36	0.51
1:C:392:PRO:CG	1:C:584:THR:HG23	2.41	0.51
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.11	0.51
1:C:514:LEU:HB3	1:C:541:MET:CE	2.41	0.51
1:D:755:GLU:HB3	1:D:759:SER:OG	2.09	0.51
1:A:599:ARG:O	1:A:603:GLU:HG3	2.10	0.51
1:B:142:ILE:HG22	1:B:143:ASP:N	2.24	0.51
1:B:188:TYR:CE2	1:B:190:PRO:HB3	2.45	0.51
1:B:194:GLU:OE1	1:B:229:ARG:NH2	2.43	0.51
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.45	0.51
1:A:506:PRO:HB2	1:A:535:ALA:HA	1.93	0.51
1:A:836:ARG:NH1	1:A:864:HIS:O	2.44	0.51
1:B:186:ILE:CG2	1:B:187:ILE:N	2.74	0.51
1:B:216:TRP:CZ2	1:B:293:ILE:HG21	2.46	0.51
1:C:298:LEU:O	1:C:299:ASN:HB2	2.10	0.51
1:D:280:PHE:CE1	1:D:561:LEU:HD11	2.46	0.51
1:D:280:PHE:HB2	1:D:340:PHE:CZ	2.46	0.51
3:L:103:DG:H2''	3:L:104:DG:OP2	2.11	0.51
1:A:255:ASN:ND2	1:A:257:TYR:CD2	2.79	0.51
1:C:152:LEU:HD22	1:C:160:GLU:HA	1.93	0.51
1:D:516:VAL:HG12	1:D:517:ASP:H	1.75	0.51
2:G:8:DT:H2''	2:G:9:DG:C8	2.45	0.51
1:A:15:ILE:HG12	1:A:65:MET:HE1	1.93	0.51
1:A:150:ASP:CG	1:A:317:HIS:HE2	2.18	0.51
1:B:502:ALA:HB1	1:B:535:ALA:HB1	1.93	0.51
1:B:898:PHE:HA	1:B:901:PHE:HD1	1.75	0.51
1:C:454:TYR:CE2	1:C:462:MET:HE3	2.45	0.51
1:C:516:VAL:HG21	1:C:522:PHE:CE1	2.45	0.51
1:C:858:ILE:O	1:C:861:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:PHE:HA	1:D:55:LYS:O	2.10	0.51
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.36	0.50
1:A:588:THR:O	1:A:591:GLN:HB2	2.11	0.50
1:A:653:LYS:HD2	1:A:653:LYS:C	2.36	0.50
1:B:834:PRO:HD2	1:B:871:LEU:HD13	1.92	0.50
1:C:163:SER:HB3	1:C:166:ILE:HB	1.92	0.50
1:D:275:ASP:O	1:D:279:LYS:HB2	2.11	0.50
1:D:726:LYS:HG3	1:D:726:LYS:O	2.10	0.50
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.11	0.50
1:A:514:LEU:HD13	1:A:529:LYS:NZ	2.27	0.50
1:B:445:ALA:HB2	1:B:596:TRP:CH2	2.46	0.50
1:B:597:ILE:HD12	1:B:683:MET:SD	2.50	0.50
1:C:38:PHE:HB2	1:C:83:LEU:HB2	1.92	0.50
1:C:109:ARG:HD2	1:C:209:THR:O	2.11	0.50
1:C:144:ASP:O	1:C:185:LYS:HD3	2.11	0.50
1:C:506:PRO:CB	1:C:535:ALA:HB2	2.41	0.50
1:D:150:ASP:OD1	1:D:321:ILE:HG12	2.11	0.50
1:D:305:TYR:CZ	1:D:312:LEU:HD22	2.47	0.50
1:A:277:TYR:CE2	1:A:293:ILE:HD12	2.46	0.50
1:A:509:SER:CA	1:A:534:SER:HB3	2.41	0.50
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.25	0.50
1:B:319:ARG:HG2	1:B:319:ARG:NH1	2.25	0.50
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.26	0.50
1:C:142:ILE:HA	4:C:915:HOH:O	2.11	0.50
1:C:475:ILE:HD13	1:C:566:LEU:HD22	1.92	0.50
1:D:388:VAL:O	1:D:390:PRO:HD3	2.11	0.50
1:A:197:LEU:HD23	1:A:198:LEU:N	2.27	0.50
1:A:689:ALA:HB1	1:A:711:ASN:O	2.11	0.50
1:B:260:ARG:NH1	1:B:260:ARG:HG2	2.26	0.50
1:B:415:LEU:O	1:B:419:ILE:HG13	2.10	0.50
1:B:668:ARG:NH1	1:B:668:ARG:CG	2.71	0.50
1:B:708:TYR:CE1	1:B:728:MET:HB3	2.47	0.50
1:C:273:TYR:HA	1:C:276:LEU:HB2	1.94	0.50
1:C:302:LYS:HD3	1:C:303:LEU:H	1.75	0.50
1:D:519:ARG:HG3	1:D:519:ARG:NH1	2.24	0.50
1:A:17:GLU:OE2	1:A:29:ARG:NH1	2.44	0.50
1:A:362:ILE:CG1	1:A:572:ASN:HD22	2.24	0.50
1:B:728:MET:CG	3:H:113:DC:H5'	2.39	0.50
1:C:333:GLN:O	1:C:336:ALA:HB3	2.11	0.50
1:D:82:ALA:H	1:D:382:GLN:NE2	2.09	0.50
1:D:164:ILE:HD13	1:D:164:ILE:N	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ILE:HD13	1:D:182:ILE:C	2.36	0.50
1:D:300:VAL:CG1	1:D:301:GLY:N	2.74	0.50
1:D:403:ARG:HH22	1:D:889:LEU:CD2	2.24	0.50
1:D:576:ARG:O	1:D:576:ARG:HG3	2.11	0.50
1:D:741:VAL:O	1:D:744:ALA:N	2.45	0.50
1:D:818:ASN:HA	1:D:857:LEU:CD1	2.42	0.50
1:A:23:ASN:HD22	1:A:25:ARG:HH22	1.58	0.50
1:B:483:LYS:CB	1:B:483:LYS:NZ	2.75	0.50
1:C:114:ASP:HB3	1:C:328:VAL:CG2	2.42	0.50
1:C:436:VAL:HG13	1:C:436:VAL:O	2.11	0.50
1:D:550:VAL:HA	1:D:553:MET:HB3	1.94	0.50
1:A:64:ASN:C	1:A:64:ASN:ND2	2.69	0.50
1:A:693:LEU:HD12	1:A:694:GLY:H	1.77	0.50
1:A:835:LEU:HD12	1:A:844:LYS:C	2.36	0.50
1:B:786:ASN:O	1:B:787:ASN:HB2	2.12	0.50
1:C:109:ARG:HH12	1:C:208:LYS:HD2	1.73	0.50
1:C:449:ARG:NH1	1:C:452:ASP:HA	2.26	0.50
1:C:642:ARG:CZ	1:C:646:HIS:HB3	2.41	0.50
1:D:825:VAL:HG12	1:D:826:GLU:N	2.26	0.50
1:D:846:ILE:HD11	1:D:862:VAL:CG1	2.39	0.50
2:G:6:DA:H2"	2:G:7:DA:H5"	1.94	0.50
1:A:145:ARG:HB2	1:A:147:TYR:HE1	1.76	0.50
1:A:221:PHE:O	1:A:222:ALA:C	2.54	0.50
1:A:803:PHE:O	1:A:845:CYS:SG	2.68	0.50
1:B:687:ALA:HB2	1:B:715:MET:CE	2.40	0.50
1:B:775:ASN:HB3	1:B:778:SER:OG	2.11	0.50
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.47	0.50
1:C:738:PRO:HG2	1:C:741:VAL:HG21	1.94	0.50
1:D:109:ARG:HD3	1:D:209:THR:O	2.11	0.50
1:D:514:LEU:HD12	1:D:541:MET:HE1	1.94	0.50
1:D:770:GLU:O	1:D:770:GLU:HG2	2.11	0.50
1:D:839:ASN:N	1:D:839:ASN:ND2	2.59	0.50
3:H:112:DT:H73	4:H:47:HOH:O	2.12	0.50
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.47	0.50
1:D:131:HIS:HB3	1:D:132:PRO:HD2	1.93	0.50
1:D:493:GLN:HB2	1:D:549:GLU:OE2	2.11	0.50
1:D:502:ALA:HB3	1:D:538:LEU:HD21	1.94	0.50
1:A:219:GLU:O	1:A:219:GLU:HG2	2.12	0.49
1:A:730:LEU:HD22	1:A:883:PHE:CE1	2.46	0.49
1:C:197:LEU:HD23	1:C:197:LEU:C	2.37	0.49
1:C:338:ARG:O	1:C:339:GLN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.34	0.49
1:D:191:PHE:CB	1:D:197:LEU:HB2	2.42	0.49
1:D:321:ILE:HD12	1:D:321:ILE:N	2.27	0.49
1:A:422:GLN:O	1:A:676:ASN:HB3	2.12	0.49
1:A:555:ALA:HB1	1:A:559:ARG:NH1	2.27	0.49
1:C:231:LYS:HE2	1:C:232:ASN:N	2.27	0.49
1:C:461:MET:CE	1:C:581:ARG:HD2	2.42	0.49
1:D:458:PRO:HG3	1:D:674:MET:CE	2.42	0.49
1:D:458:PRO:HG3	1:D:674:MET:HE3	1.93	0.49
1:D:663:ILE:O	1:D:664:ASP:C	2.54	0.49
1:D:835:LEU:HD21	1:D:846:ILE:HG23	1.93	0.49
1:B:129:ALA:HB1	1:B:229:ARG:CG	2.42	0.49
1:B:245:HIS:CD2	1:B:267:GLY:HA3	2.47	0.49
1:B:247:LYS:HE3	1:B:266:PHE:CE2	2.47	0.49
1:B:413:THR:O	1:B:414:SER:C	2.55	0.49
1:D:412:LEU:HD21	1:D:683:MET:CE	2.42	0.49
1:D:420:ILE:O	1:D:424:ASN:N	2.44	0.49
1:A:420:ILE:HG12	1:A:586:ILE:CD1	2.42	0.49
1:B:739:LYS:HE2	1:B:742:GLN:NE2	2.26	0.49
1:C:66:ARG:HD2	1:C:66:ARG:O	2.12	0.49
1:C:109:ARG:HE	1:C:142:ILE:HD12	1.78	0.49
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.44	0.49
1:C:191:PHE:CE2	1:C:197:LEU:HA	2.48	0.49
1:A:51:ASP:OD1	1:A:53:TYR:N	2.44	0.49
1:A:94:SER:HB3	1:A:371:ASN:OD1	2.12	0.49
1:A:472:PRO:HA	1:A:475:ILE:HG13	1.94	0.49
1:A:509:SER:HB3	1:A:534:SER:HB3	1.95	0.49
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.93	0.49
1:A:803:PHE:CZ	1:A:845:CYS:HB3	2.47	0.49
1:B:475:ILE:C	1:B:475:ILE:HD13	2.38	0.49
1:B:644:THR:HG21	1:C:77:ASP:OD2	2.12	0.49
1:B:748:CYS:O	1:B:752:MET:HG3	2.12	0.49
1:C:458:PRO:CG	1:C:592:MET:SD	3.01	0.49
1:D:164:ILE:O	1:D:168:ALA:N	2.40	0.49
1:D:296:PHE:CD1	1:D:297:GLU:N	2.80	0.49
1:D:405:LYS:O	1:D:691:PRO:HD3	2.13	0.49
1:A:195:LYS:HE2	1:A:233:ILE:HG23	1.93	0.49
1:A:514:LEU:CD1	1:A:526:ILE:HG23	2.40	0.49
1:B:722:GLU:OE1	1:B:722:GLU:HA	2.12	0.49
1:B:808:ILE:O	1:B:812:ASN:ND2	2.45	0.49
1:D:180:SER:O	1:D:182:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:HD12	1:D:536:LYS:N	2.27	0.49
3:L:111:DT:H2''	3:L:112:DT:C6	2.47	0.49
1:A:511:ASP:OD2	1:A:512:GLU:N	2.45	0.49
1:A:747:GLU:OE2	1:A:747:GLU:HA	2.13	0.49
1:A:782:VAL:CG1	1:A:783:SER:N	2.75	0.49
1:B:273:TYR:CZ	1:B:340:PHE:HB2	2.48	0.49
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.42	0.49
1:B:773:GLN:NE2	1:B:773:GLN:H	2.10	0.49
1:C:83:LEU:HD22	1:C:83:LEU:N	2.28	0.49
1:D:223:ILE:HB	1:D:224:PRO:CD	2.40	0.49
1:D:289:SER:O	1:D:293:ILE:HG13	2.13	0.49
1:D:578:TYR:C	1:D:578:TYR:CD1	2.90	0.49
2:G:4:CTG:H2'	2:G:5:DG:C8	2.47	0.49
3:L:110:DA:H1'	3:L:111:DT:H5''	1.93	0.49
1:B:329:TYR:O	1:B:330:ARG:C	2.55	0.49
1:B:876:PHE:O	1:B:879:PRO:HG2	2.11	0.49
1:C:110:VAL:HB	1:C:141:SER:HB3	1.94	0.49
1:C:726:LYS:HG3	1:C:728:MET:CE	2.42	0.49
1:D:162:TRP:CZ3	1:D:188:TYR:HB2	2.48	0.49
1:D:180:SER:HA	1:D:183:ILE:HG13	1.95	0.49
1:D:795:GLY:HA3	1:D:813:ARG:HD3	1.94	0.49
1:A:61:LEU:HD22	1:A:61:LEU:C	2.38	0.49
1:A:730:LEU:HB3	1:A:883:PHE:HZ	1.75	0.49
1:B:217:ASN:N	1:B:274:ILE:HG21	2.16	0.49
1:B:233:ILE:HG22	1:B:233:ILE:O	2.12	0.49
1:B:278:LYS:HE2	1:B:288:TYR:CD2	2.47	0.49
1:B:362:ILE:HG12	2:G:3:DT:C5'	2.43	0.49
1:B:858:ILE:HB	1:B:862:VAL:HG23	1.94	0.49
1:D:41:CYS:HB3	1:D:57:CYS:CA	2.40	0.49
1:D:157:GLY:O	1:D:313:ARG:NH1	2.46	0.49
1:D:491:ALA:O	1:D:495:ASN:HB2	2.13	0.49
1:D:668:ARG:HG2	1:D:679:HIS:ND1	2.28	0.49
1:A:868:TYR:O	1:A:869:THR:C	2.55	0.49
1:B:398:GLU:OE2	1:B:705:LYS:HE3	2.13	0.49
1:B:530:ILE:HG13	1:B:531:LYS:N	2.28	0.49
1:B:887:ALA:O	1:B:888:LYS:HB2	2.12	0.49
1:C:495:ASN:HB3	1:C:522:PHE:CD2	2.48	0.49
1:D:419:ILE:HG23	1:D:589:PHE:CD1	2.48	0.49
1:A:97:TYR:O	1:A:352:LYS:HE3	2.13	0.48
1:A:138:HIS:C	1:A:138:HIS:CD2	2.90	0.48
1:A:741:VAL:C	1:A:743:LYS:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HB2	1:B:130:LYS:NZ	2.28	0.48
1:B:139:TYR:CG	1:B:140:ASP:N	2.80	0.48
1:B:270:VAL:O	1:B:270:VAL:HG13	2.12	0.48
1:C:182:ILE:HD13	1:C:329:TYR:CG	2.48	0.48
1:C:324:ASN:O	1:C:328:VAL:HG23	2.13	0.48
1:C:691:PRO:HD3	1:C:699:GLY:HA3	1.94	0.48
1:D:810:THR:O	1:D:841:PHE:HE1	1.95	0.48
1:A:4:PHE:N	1:A:4:PHE:HD1	2.11	0.48
1:C:482:ARG:CZ	1:C:560:LYS:HB2	2.43	0.48
1:D:582:ASN:O	1:D:585:ALA:HB3	2.12	0.48
3:L:104:DG:C2'	3:L:105:DC:H5''	2.39	0.48
1:A:380:ILE:HD12	1:A:576:ARG:NE	2.27	0.48
1:B:273:TYR:HA	1:B:276:LEU:HD12	1.95	0.48
1:C:194:GLU:O	1:C:195:LYS:C	2.55	0.48
1:C:203:ASN:HA	1:C:206:GLN:HG2	1.94	0.48
1:C:831:TYR:CE2	1:C:851:GLY:N	2.80	0.48
1:D:96:THR:C	1:D:97:TYR:CD1	2.91	0.48
1:D:506:PRO:O	1:D:507:ASN:ND2	2.44	0.48
1:A:6:LEU:CD1	1:A:26:GLU:HG3	2.43	0.48
1:A:296:PHE:HD2	1:A:297:GLU:CG	2.26	0.48
1:A:303:LEU:HB2	1:A:323:TYR:HD1	1.78	0.48
1:A:536:LYS:HD3	1:A:536:LYS:C	2.38	0.48
1:A:702:TRP:NE1	1:A:708:TYR:HD1	2.11	0.48
1:B:110:VAL:H	1:B:141:SER:HB3	1.79	0.48
1:B:313:ARG:HG2	1:B:314:GLU:OE1	2.12	0.48
1:B:775:ASN:ND2	1:B:777:ILE:H	2.12	0.48
1:D:2:LYS:HG2	1:D:3:GLU:H	1.78	0.48
1:D:36:SER:HB3	1:D:59:ARG:NH1	2.28	0.48
1:D:144:ASP:OD1	1:D:185:LYS:HE3	2.14	0.48
1:D:559:ARG:O	1:D:562:LEU:HB3	2.14	0.48
1:A:279:LYS:NZ	2:E:3:DT:H71	2.24	0.48
1:A:506:PRO:HB2	1:A:535:ALA:CB	2.43	0.48
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.95	0.48
1:A:870:VAL:O	1:A:874:LYS:HG2	2.14	0.48
1:B:268:ILE:HG22	1:B:269:SER:N	2.29	0.48
1:B:362:ILE:HG12	2:G:3:DT:H5'	1.94	0.48
1:B:499:ILE:HG21	1:B:530:ILE:HD12	1.95	0.48
1:B:771:PHE:HD1	1:B:774:LEU:HD12	1.79	0.48
1:C:204:PHE:O	1:C:208:LYS:HB2	2.14	0.48
1:C:426:SER:OG	1:C:427:PRO:HD2	2.14	0.48
1:D:273:TYR:HA	1:D:276:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:SER:HB2	1:D:363:LYS:HB3	1.95	0.48
2:G:8:DT:H2'	2:G:9:DG:C8	2.48	0.48
1:A:126:PRO:HA	1:A:225:TYR:CD1	2.49	0.48
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.95	0.48
1:C:661:PRO:O	1:C:662:ALA:C	2.55	0.48
1:D:848:TRP:CB	1:D:854:ILE:HB	2.44	0.48
1:A:63:ALA:HB3	1:A:67:ASP:OD1	2.14	0.48
1:A:836:ARG:HH12	1:A:865:TRP:HA	1.73	0.48
1:B:52:ILE:HD12	1:B:428:GLU:HB3	1.94	0.48
1:B:119:SER:CB	1:B:124:PRO:HG3	2.44	0.48
1:B:324:ASN:O	1:B:327:ALA:HB3	2.14	0.48
1:C:312:LEU:O	1:C:313:ARG:C	2.55	0.48
1:C:499:ILE:HG21	1:C:542:LEU:HB2	1.94	0.48
1:D:482:ARG:C	1:D:484:GLU:N	2.68	0.48
3:F:105:DC:H2''	3:F:106:DT:O5'	2.14	0.48
1:A:45:GLN:O	1:A:46:ALA:C	2.56	0.48
1:A:195:LYS:HE2	1:A:233:ILE:CG2	2.44	0.48
1:A:482:ARG:HE	1:A:556:GLN:HE21	1.61	0.48
1:A:737:THR:O	1:A:738:PRO:O	2.31	0.48
1:B:428:GLU:OE2	1:B:428:GLU:N	2.39	0.48
1:B:486:LYS:HB3	1:B:556:GLN:NE2	2.28	0.48
1:B:772:ARG:CZ	1:B:868:TYR:HB2	2.44	0.48
1:B:796:PHE:HD1	1:B:813:ARG:NH1	2.10	0.48
1:B:835:LEU:HA	1:B:866:MET:HA	1.95	0.48
1:C:109:ARG:HH11	1:C:208:LYS:HA	1.78	0.48
1:C:176:ASP:O	1:C:177:GLU:CB	2.60	0.48
1:D:805:ILE:O	1:D:809:LEU:HG	2.14	0.48
1:D:835:LEU:HD13	1:D:839:ASN:OD1	2.14	0.48
1:B:312:LEU:HD12	1:B:320:TYR:HD1	1.78	0.48
1:B:713:TRP:CZ3	1:B:723:PRO:HD3	2.48	0.48
1:B:837:GLU:CG	1:B:838:GLY:N	2.76	0.48
1:B:894:LYS:NZ	1:B:894:LYS:CB	2.67	0.48
1:C:85:MET:CA	1:C:380:ILE:HD11	2.42	0.48
1:C:319:ARG:O	1:C:322:SER:N	2.46	0.48
1:D:437:ALA:HB3	1:D:442:TYR:CZ	2.49	0.48
3:J:105:DC:H2'	3:J:106:DT:C5	2.48	0.48
1:A:19:TYR:CE1	1:A:29:ARG:HG2	2.49	0.48
1:A:41:CYS:HB2	1:A:42:PRO:CD	2.43	0.48
1:A:641:PHE:HA	1:A:646:HIS:CD2	2.48	0.48
1:A:830:VAL:HA	1:A:848:TRP:O	2.14	0.48
1:B:142:ILE:HD12	1:B:142:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.96	0.48
1:B:898:PHE:HA	1:B:901:PHE:CD1	2.49	0.48
1:C:343:LEU:HD11	1:C:558:ASN:ND2	2.29	0.48
1:D:9:GLU:O	1:D:15:ILE:HA	2.14	0.48
1:D:136:ILE:HD11	1:D:201:TYR:CE1	2.49	0.48
1:D:159:VAL:CG1	1:D:160:GLU:H	2.20	0.48
1:D:368:ILE:HD11	1:D:562:LEU:HD11	1.96	0.48
1:D:727:ILE:HG23	1:D:730:LEU:HD12	1.95	0.48
1:D:776:TYR:O	1:D:779:ILE:CD1	2.61	0.48
1:A:846:ILE:O	1:A:846:ILE:HG13	2.14	0.47
1:B:408:MET:HE1	1:B:655:ALA:CB	2.44	0.47
1:B:901:PHE:CZ	1:D:650:PHE:HZ	2.32	0.47
1:B:901:PHE:HZ	1:D:650:PHE:HZ	1.59	0.47
1:C:87:ASP:OD2	1:C:90:LEU:HD13	2.13	0.47
1:C:109:ARG:NH1	1:C:208:LYS:HD2	2.29	0.47
1:C:115:ILE:HG13	1:C:116:GLU:N	2.27	0.47
1:D:442:TYR:CB	1:D:592:MET:HE3	2.36	0.47
1:D:592:MET:HE1	1:D:674:MET:HE1	1.95	0.47
1:A:280:PHE:CD2	1:A:343:LEU:HD21	2.49	0.47
1:A:780:ALA:HA	1:A:833:LEU:CD2	2.44	0.47
1:B:405:LYS:HA	1:B:698:ILE:O	2.14	0.47
1:B:517:ASP:C	1:B:519:ARG:H	2.22	0.47
1:B:693:LEU:HA	4:B:938:HOH:O	2.14	0.47
1:B:841:PHE:HE1	1:B:858:ILE:HG21	1.79	0.47
1:C:454:TYR:HB3	1:C:463:TYR:O	2.14	0.47
1:D:218:VAL:HG12	1:D:223:ILE:HG13	1.97	0.47
1:D:410:PHE:HB3	1:D:683:MET:HG2	1.96	0.47
1:D:420:ILE:HD12	1:D:420:ILE:N	2.29	0.47
1:D:815:ILE:CG2	1:D:858:ILE:HD13	2.41	0.47
1:A:606:ASN:HD21	1:A:613:GLY:HA2	1.76	0.47
1:A:846:ILE:HD12	1:A:847:ALA:N	2.29	0.47
1:A:868:TYR:O	1:A:871:LEU:N	2.46	0.47
1:B:228:ASN:HA	1:B:231:LYS:HE3	1.95	0.47
1:B:466:ASP:OD2	1:B:467:ARG:N	2.47	0.47
1:B:900:MET:O	1:D:635:LYS:HE3	2.14	0.47
1:C:55:LYS:N	1:C:55:LYS:HE2	2.29	0.47
1:D:37:LEU:HD11	1:D:72:ILE:HD11	1.96	0.47
1:D:116:GLU:HG2	1:D:324:ASN:OD1	2.14	0.47
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.96	0.47
1:D:461:MET:HA	1:D:461:MET:HE3	1.96	0.47
3:J:112:DT:H2'	3:J:113:DC:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:HA3	1:A:107:LYS:HE3	1.96	0.47
1:A:864:HIS:HD2	1:A:865:TRP:NE1	2.12	0.47
1:B:109:ARG:HD2	1:B:140:ASP:OD2	2.14	0.47
1:B:491:ALA:O	1:B:495:ASN:N	2.45	0.47
1:D:489:MET:O	1:D:493:GLN:HG2	2.13	0.47
1:D:833:LEU:HD22	1:D:834:PRO:HD2	1.96	0.47
1:D:647:TRP:CZ3	1:D:651:LEU:HD12	2.50	0.47
1:A:522:PHE:HB2	1:A:527:LYS:HE3	1.96	0.47
1:B:145:ARG:HG2	1:B:187:ILE:HD12	1.96	0.47
1:B:309:ILE:HA	1:B:312:LEU:HB2	1.96	0.47
1:B:486:LYS:O	1:B:490:LEU:HB2	2.15	0.47
1:B:594:LEU:HD11	1:B:625:ILE:CG2	2.45	0.47
1:C:135:ALA:C	1:C:136:ILE:HG13	2.38	0.47
1:D:113:PHE:CZ	1:D:222:ALA:HB1	2.49	0.47
1:D:330:ARG:HD3	1:D:333:GLN:OE1	2.15	0.47
1:D:578:TYR:CD1	1:D:579:ASP:N	2.82	0.47
3:L:105:DC:H2'	3:L:106:DT:H72	1.97	0.47
1:A:255:ASN:ND2	1:A:257:TYR:HD2	2.12	0.47
1:A:404:TYR:CE1	1:A:618:LEU:HD13	2.50	0.47
1:A:602:ASN:HD21	1:A:616:PHE:H	1.62	0.47
1:B:103:TYR:N	1:B:103:TYR:CD1	2.81	0.47
1:B:186:ILE:HG22	1:B:187:ILE:H	1.79	0.47
1:B:247:LYS:HE3	1:B:266:PHE:CZ	2.50	0.47
1:B:330:ARG:HA	1:B:333:GLN:OE1	2.14	0.47
1:B:471:VAL:N	1:B:472:PRO:HD2	2.30	0.47
1:B:891:TYR:CD2	1:B:891:TYR:N	2.82	0.47
1:C:7:THR:OG1	1:C:7:THR:O	2.31	0.47
1:C:118:THR:OG1	1:C:313:ARG:HG3	2.15	0.47
1:C:134:ASP:O	1:C:135:ALA:HB2	2.15	0.47
1:C:413:THR:O	1:C:414:SER:C	2.57	0.47
1:C:506:PRO:C	1:C:507:ASN:HD22	2.23	0.47
1:C:789:ALA:O	1:C:791:TYR:N	2.48	0.47
1:D:117:VAL:HG21	1:D:225:TYR:CE1	2.50	0.47
1:D:469:GLY:HA3	1:D:472:PRO:HD2	1.96	0.47
1:D:514:LEU:H	1:D:541:MET:CE	2.27	0.47
1:D:741:VAL:HG13	1:D:876:PHE:HD1	1.80	0.47
1:D:874:LYS:HG3	1:D:875:THR:N	2.29	0.47
1:A:191:PHE:HA	4:A:928:HOH:O	2.15	0.47
1:A:217:ASN:HA	1:A:272:ASP:OD2	2.14	0.47
1:A:458:PRO:HG3	1:A:592:MET:SD	2.54	0.47
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:PHE:CE1	1:B:659:MET:HG3	2.50	0.47
1:C:572:ASN:HD21	1:C:574:TRP:HB2	1.80	0.47
1:D:113:PHE:HE1	1:D:218:VAL:HG13	1.79	0.47
1:D:508:LEU:CD2	1:D:534:SER:HB2	2.45	0.47
1:D:698:ILE:HG12	1:D:752:MET:O	2.15	0.47
1:D:825:VAL:HB	1:D:828:GLU:HG2	1.97	0.47
3:L:110:DA:C2'	3:L:111:DT:C5'	2.91	0.47
1:A:21:ASP:OD1	1:A:25:ARG:NH1	2.48	0.47
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.44	0.47
1:A:43:GLU:N	1:A:43:GLU:OE2	2.47	0.47
1:A:83:LEU:HD12	1:A:83:LEU:H	1.77	0.47
1:A:105:HIS:ND1	1:A:106:THR:N	2.63	0.47
1:A:433:THR:HA	1:A:460:GLY:O	2.15	0.47
1:A:786:ASN:HD22	1:A:786:ASN:N	2.12	0.47
1:B:472:PRO:O	1:B:475:ILE:HG22	2.15	0.47
1:B:898:PHE:N	1:B:898:PHE:CD1	2.83	0.47
1:C:606:ASN:HB3	1:C:611:THR:O	2.15	0.47
1:D:277:TYR:HE1	1:D:338:ARG:CZ	2.28	0.47
1:D:345:LEU:HD23	1:D:355:ILE:HG21	1.95	0.47
1:D:777:ILE:HD11	1:D:853:GLU:HA	1.95	0.47
1:D:892:GLU:O	1:D:894:LYS:HG3	2.15	0.47
3:J:105:DC:C2'	3:J:106:DT:C6	2.98	0.47
3:J:110:DA:C2'	3:J:111:DT:H5''	2.45	0.47
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.97	0.47
1:A:643:ASP:C	1:A:693:LEU:HD23	2.39	0.47
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.79	0.47
1:B:644:THR:HG23	1:B:645:ASN:H	1.79	0.47
1:C:482:ARG:NH1	1:C:556:GLN:HE21	2.06	0.47
1:D:207:GLN:HG2	1:D:208:LYS:HD2	1.96	0.47
1:D:342:ASN:OD1	1:D:554:THR:HG21	2.15	0.47
1:D:793:VAL:CG2	1:D:796:PHE:HB2	2.44	0.47
1:A:606:ASN:ND2	1:A:613:GLY:N	2.60	0.46
1:B:71:TRP:CE2	1:B:75:MET:HE3	2.50	0.46
1:B:197:LEU:HD23	1:B:197:LEU:O	2.15	0.46
1:B:516:VAL:HG13	1:B:544:ARG:NH1	2.26	0.46
1:C:221:PHE:O	1:C:222:ALA:C	2.58	0.46
1:C:474:GLU:O	1:C:477:LYS:N	2.44	0.46
1:D:414:SER:O	1:D:417:PRO:HD2	2.14	0.46
3:H:110:DA:H2''	3:H:111:DT:H5''	1.97	0.46
1:A:406:TYR:CD2	1:A:633:ILE:HG13	2.50	0.46
1:A:653:LYS:HD3	1:A:657:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:CD	1:A:866:MET:O	2.64	0.46
1:B:731:GLU:HA	1:B:734:LYS:HG2	1.97	0.46
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.50	0.46
1:D:6:LEU:HG	1:D:19:TYR:HA	1.97	0.46
1:D:154:SER:HB3	1:D:155:PRO:HD2	1.96	0.46
1:D:345:LEU:O	1:D:349:TYR:HD1	1.98	0.46
1:D:373:LEU:CD1	1:D:380:ILE:HG22	2.43	0.46
2:G:17:DC:H2''	2:G:18:DG:O5'	2.15	0.46
1:A:493:GLN:O	1:A:497:GLU:HG2	2.15	0.46
1:B:48:LYS:O	1:B:377:ASN:HB3	2.15	0.46
1:B:271:LEU:HB3	1:B:276:LEU:CD1	2.39	0.46
1:B:655:ALA:HA	1:B:659:MET:HB2	1.98	0.46
1:B:790:LYS:HE3	1:B:791:TYR:CZ	2.50	0.46
1:D:280:PHE:HE1	1:D:561:LEU:HD11	1.80	0.46
1:D:699:GLY:C	1:D:753:LEU:HD22	2.40	0.46
1:D:764:PHE:CE1	1:D:876:PHE:HE2	2.33	0.46
1:A:297:GLU:C	1:A:298:LEU:HD12	2.41	0.46
1:A:409:SER:O	1:A:686:GLU:HB2	2.14	0.46
1:B:205:TRP:NE1	1:B:242:LEU:O	2.48	0.46
1:B:235:GLY:O	1:B:236:GLU:C	2.58	0.46
1:C:199:MET:O	1:C:202:LEU:HB3	2.16	0.46
1:C:671:CYS:SG	1:C:676:ASN:HB2	2.55	0.46
1:D:95:ASP:O	1:D:97:TYR:N	2.49	0.46
1:D:498:ILE:O	1:D:498:ILE:HG22	2.14	0.46
1:D:725:LEU:H	1:D:725:LEU:HD22	1.81	0.46
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.51	0.46
1:A:294:SER:O	1:A:298:LEU:CD1	2.63	0.46
1:B:415:LEU:HD11	1:B:419:ILE:HD11	1.98	0.46
1:B:516:VAL:HG22	1:B:517:ASP:H	1.80	0.46
1:B:863:LEU:HD12	1:B:866:MET:HE3	1.97	0.46
1:D:109:ARG:HH21	1:D:208:LYS:HB3	1.70	0.46
1:A:692:PRO:HD2	1:A:695:SER:OG	2.16	0.46
1:A:741:VAL:C	1:A:743:LYS:H	2.22	0.46
1:A:841:PHE:O	1:A:842:GLY:C	2.58	0.46
1:A:878:LYS:N	1:A:879:PRO:HD2	2.30	0.46
1:B:231:LYS:HB2	1:B:239:ALA:HB2	1.97	0.46
1:B:494:ARG:C	1:B:496:GLY:H	2.23	0.46
1:B:533:LEU:HG	1:B:534:SER:H	1.80	0.46
1:B:831:TYR:HD2	1:B:848:TRP:NE1	2.13	0.46
1:C:148:VAL:C	1:C:149:PHE:HD1	2.24	0.46
1:C:214:THR:HG21	1:C:341:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:SER:O	1:C:415:LEU:C	2.57	0.46
1:C:520:PHE:O	1:C:521:ASP:C	2.58	0.46
1:C:594:LEU:O	1:C:597:ILE:HG22	2.16	0.46
1:D:218:VAL:HA	1:D:222:ALA:CB	2.41	0.46
1:D:296:PHE:CD1	1:D:296:PHE:C	2.94	0.46
1:D:469:GLY:CA	1:D:472:PRO:HD2	2.46	0.46
1:A:362:ILE:HD12	1:A:569:ALA:CB	2.45	0.46
1:A:562:LEU:O	1:A:563:ILE:C	2.56	0.46
1:B:146:PHE:N	1:B:146:PHE:CD1	2.83	0.46
1:C:686:GLU:HG3	1:C:715:MET:HE3	1.95	0.46
1:C:707:ARG:HB3	1:C:730:LEU:HD23	1.98	0.46
1:D:202:LEU:HD11	1:D:241:ARG:HB3	1.98	0.46
1:D:361:PRO:HB3	1:D:565:SER:HB2	1.97	0.46
1:C:139:TYR:CD2	1:C:332:LEU:HD21	2.51	0.46
1:C:489:MET:SD	1:C:553:MET:HE2	2.56	0.46
1:C:559:ARG:HD3	1:C:559:ARG:HA	1.78	0.46
1:C:839:ASN:C	1:C:841:PHE:H	2.24	0.46
1:D:218:VAL:CG1	1:D:223:ILE:HG13	2.46	0.46
1:D:230:ILE:HG21	1:D:239:ALA:HA	1.97	0.46
1:D:241:ARG:C	1:D:243:SER:H	2.23	0.46
1:D:597:ILE:CG2	1:D:683:MET:HE1	2.35	0.46
1:A:36:SER:O	1:A:37:LEU:HD23	2.15	0.46
1:A:113:PHE:CE2	1:A:222:ALA:HB1	2.51	0.46
1:A:129:ALA:HB1	1:A:229:ARG:HG2	1.98	0.46
1:A:218:VAL:HG22	1:A:223:ILE:HG13	1.97	0.46
1:A:426:SER:OG	1:A:427:PRO:HD2	2.16	0.46
1:A:685:ARG:HD2	1:A:688:ILE:HD11	1.97	0.46
1:B:505:ASN:HB3	1:B:535:ALA:HB3	1.97	0.46
1:B:800:LYS:O	1:B:800:LYS:HG2	2.14	0.46
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.98	0.46
1:B:887:ALA:CB	1:B:889:LEU:HD12	2.46	0.46
2:E:16:DG:H2''	2:E:17:DC:H5''	1.98	0.46
1:A:293:ILE:O	1:A:293:ILE:HG22	2.15	0.46
1:A:296:PHE:HD2	1:A:297:GLU:HG2	1.81	0.46
1:B:41:CYS:HB2	1:B:42:PRO:HD2	1.98	0.46
1:B:654:PHE:O	1:B:658:ARG:HB2	2.16	0.46
1:B:901:PHE:CD2	1:D:608:VAL:HG12	2.51	0.46
1:C:17:GLU:OE1	1:C:97:TYR:OH	2.23	0.46
1:C:17:GLU:HG2	1:C:18:ARG:N	2.30	0.46
1:C:109:ARG:HH11	1:C:208:LYS:CA	2.29	0.46
1:D:74:ARG:O	1:D:77:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:LYS:C	1:D:562:LEU:N	2.74	0.46
1:D:560:LYS:O	1:D:563:ILE:N	2.49	0.46
1:A:6:LEU:HD12	1:A:26:GLU:HG3	1.98	0.45
1:A:602:ASN:HD22	1:A:616:PHE:HB2	1.80	0.45
1:A:643:ASP:HA	1:A:693:LEU:HD23	1.97	0.45
1:B:61:LEU:CD2	1:B:62:PHE:H	2.29	0.45
1:B:168:ALA:HA	1:B:178:VAL:HG12	1.97	0.45
1:C:488:TYR:HB3	1:C:519:ARG:HG2	1.98	0.45
1:C:642:ARG:N	1:C:642:ARG:CD	2.71	0.45
1:C:726:LYS:HG3	1:C:728:MET:HE3	1.97	0.45
1:D:14:SER:HA	1:D:32:GLU:HA	1.98	0.45
1:A:213:LEU:HD12	1:A:223:ILE:HD11	1.99	0.45
1:A:402:ASN:HB3	1:A:404:TYR:CE2	2.50	0.45
1:A:685:ARG:HH11	1:A:688:ILE:HG13	1.79	0.45
1:B:170:LEU:N	1:B:170:LEU:HD12	2.31	0.45
1:B:503:LEU:O	1:B:504:HIS:C	2.58	0.45
1:C:116:GLU:HG3	1:C:324:ASN:HB2	1.98	0.45
1:C:136:ILE:HG22	1:C:137:THR:N	2.31	0.45
1:C:151:LEU:CD2	1:C:154:SER:HB3	2.45	0.45
1:C:454:TYR:HB2	1:C:462:MET:HG2	1.98	0.45
1:C:768:GLU:HG2	1:C:872:LEU:HD21	1.97	0.45
1:D:214:THR:HG22	1:D:273:TYR:HB2	1.97	0.45
1:D:576:ARG:HB2	1:D:576:ARG:CZ	2.46	0.45
1:D:793:VAL:O	1:D:793:VAL:HG23	2.16	0.45
1:D:815:ILE:HG22	1:D:858:ILE:CG2	2.30	0.45
1:D:187:ILE:O	1:D:187:ILE:HG12	2.15	0.45
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.51	0.45
1:A:42:PRO:O	1:A:45:GLN:N	2.43	0.45
1:A:87:ASP:OD1	1:A:363:LYS:NZ	2.32	0.45
1:A:126:PRO:HG3	1:A:221:PHE:CD1	2.51	0.45
1:B:132:PRO:HA	1:B:194:GLU:OE1	2.16	0.45
1:B:168:ALA:HA	1:B:178:VAL:CG1	2.46	0.45
1:B:736:SER:HA	1:B:782:VAL:HB	1.98	0.45
1:C:66:ARG:HD2	1:C:66:ARG:C	2.41	0.45
1:C:130:LYS:O	1:C:229:ARG:NH1	2.49	0.45
1:C:441:ASP:HB3	1:C:447:ALA:HB2	1.98	0.45
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.73	0.45
1:D:482:ARG:HG2	1:D:559:ARG:CB	2.46	0.45
1:D:644:THR:HG21	1:D:713:TRP:CZ2	2.52	0.45
1:A:186:ILE:HG22	1:A:187:ILE:N	2.30	0.45
1:A:337:LYS:O	1:A:339:GLN:OE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ALA:HA	1:A:833:LEU:HD21	1.98	0.45
1:B:104:ASP:C	1:B:104:ASP:OD2	2.58	0.45
1:B:123:PHE:CE2	1:B:126:PRO:HD3	2.51	0.45
1:B:231:LYS:CG	1:B:236:GLU:HA	2.39	0.45
1:B:374:LYS:C	1:B:376:GLN:N	2.73	0.45
1:C:142:ILE:HG22	1:C:143:ASP:OD1	2.17	0.45
1:C:572:ASN:ND2	1:C:574:TRP:H	2.15	0.45
1:C:614:GLU:OE1	1:C:631:LYS:NZ	2.49	0.45
1:C:782:VAL:HG12	1:C:783:SER:N	2.30	0.45
1:D:406:TYR:CE2	1:D:691:PRO:HD2	2.51	0.45
1:D:420:ILE:HD11	1:D:586:ILE:HD13	1.98	0.45
2:I:6:DA:H2''	2:I:7:DA:C5'	2.43	0.45
1:A:112:ASN:ND2	1:A:214:THR:HG23	2.31	0.45
1:A:408:MET:HE2	1:A:685:ARG:HG3	1.98	0.45
1:A:680:LEU:HA	1:A:682:PHE:CZ	2.52	0.45
1:B:355:ILE:O	1:B:358:VAL:HG13	2.16	0.45
1:B:389:GLN:OE1	1:B:390:PRO:HD2	2.16	0.45
1:B:445:ALA:HA	1:B:673:TYR:CE2	2.51	0.45
1:B:751:ARG:O	1:B:756:GLY:N	2.33	0.45
1:C:109:ARG:NH1	1:C:208:LYS:CA	2.78	0.45
1:C:132:PRO:HB3	1:C:229:ARG:HH21	1.82	0.45
1:C:145:ARG:HD3	1:C:185:LYS:HB3	1.99	0.45
1:C:274:ILE:CG2	1:C:275:ASP:N	2.78	0.45
1:C:458:PRO:HG3	1:C:592:MET:SD	2.57	0.45
1:D:135:ALA:C	1:D:136:ILE:HG22	2.40	0.45
1:D:180:SER:O	1:D:183:ILE:HG13	2.17	0.45
1:D:250:VAL:HG22	1:D:263:ILE:HG13	1.98	0.45
1:D:422:GLN:OE1	1:D:681:MET:HG2	2.17	0.45
1:D:443:ILE:HG22	1:D:443:ILE:O	2.17	0.45
1:D:706:LYS:NZ	1:D:706:LYS:HB2	2.31	0.45
1:A:207:GLN:C	1:A:208:LYS:HG3	2.41	0.45
1:A:221:PHE:C	1:A:224:PRO:HD2	2.42	0.45
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.47	0.45
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.99	0.45
1:A:502:ALA:C	1:A:503:LEU:HD12	2.41	0.45
1:A:819:ILE:HG13	1:A:819:ILE:O	2.17	0.45
1:B:362:ILE:HD11	1:B:572:ASN:CB	2.47	0.45
1:B:867:ASP:OD1	1:B:870:VAL:HB	2.17	0.45
1:C:42:PRO:O	1:C:43:GLU:C	2.59	0.45
1:C:251:LYS:N	1:C:262:ILE:O	2.50	0.45
1:D:62:PHE:CD2	1:D:68:ALA:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PRO:N	1:D:229:ARG:HH21	2.14	0.45
1:D:162:TRP:HZ3	1:D:188:TYR:HB2	1.81	0.45
1:D:291:ASP:O	1:D:292:TYR:C	2.60	0.45
1:D:303:LEU:O	1:D:304:LYS:C	2.59	0.45
1:D:347:MET:HE2	1:D:558:ASN:HD21	1.82	0.45
1:D:401:PRO:O	1:D:402:ASN:HB2	2.16	0.45
1:D:659:MET:O	1:D:660:GLU:C	2.59	0.45
1:A:412:LEU:HG	1:A:683:MET:HG2	1.98	0.45
1:A:467:ARG:HH11	1:A:467:ARG:CG	2.28	0.45
1:A:559:ARG:CG	1:A:559:ARG:NH1	2.74	0.45
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.51	0.45
1:A:731:GLU:OE1	1:A:731:GLU:N	2.48	0.45
1:A:775:ASN:O	1:A:778:SER:OG	2.32	0.45
1:B:597:ILE:O	1:B:601:VAL:HG23	2.17	0.45
1:C:112:ASN:HA	1:C:214:THR:O	2.17	0.45
1:C:223:ILE:CB	1:C:224:PRO:HD3	2.46	0.45
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.99	0.45
1:C:811:TYR:O	1:C:815:ILE:HG12	2.17	0.45
1:D:202:LEU:HD23	1:D:202:LEU:C	2.41	0.45
1:D:216:TRP:CB	1:D:290:LEU:HD12	2.46	0.45
1:D:296:PHE:HD1	1:D:297:GLU:N	2.15	0.45
1:D:353:ILE:HG13	1:D:354:GLN:O	2.17	0.45
1:D:777:ILE:CG2	1:D:831:TYR:HE1	2.30	0.45
1:A:194:GLU:CD	1:A:229:ARG:NH1	2.74	0.45
1:B:218:VAL:HG13	1:B:223:ILE:HG13	1.99	0.45
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.98	0.45
1:C:438:PRO:O	1:C:439:LEU:C	2.60	0.45
1:D:486:LYS:O	1:D:490:LEU:HB2	2.17	0.45
1:D:592:MET:O	1:D:593:ALA:C	2.59	0.45
1:D:605:LEU:CD2	1:D:632:ILE:HD11	2.47	0.45
3:F:109:DC:H2''	3:F:110:DA:H5'	1.98	0.45
2:G:11:DC:H2''	2:G:12:DA:C5'	2.45	0.45
1:A:503:LEU:CD1	1:A:538:LEU:HB3	2.46	0.45
1:A:511:ASP:OD1	1:A:533:LEU:HD22	2.16	0.45
1:A:548:THR:O	1:A:551:ALA:N	2.50	0.45
1:B:50:PHE:O	1:B:378:LYS:HA	2.17	0.45
1:B:202:LEU:HD21	1:B:241:ARG:CB	2.47	0.45
1:B:220:SER:C	1:B:224:PRO:HG2	2.42	0.45
1:B:530:ILE:HG13	1:B:531:LYS:H	1.82	0.45
1:B:685:ARG:NH2	1:B:714:ASP:OD1	2.50	0.45
1:C:189:MET:O	1:C:191:PHE:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLN:HB2	1:C:378:LYS:HG3	1.99	0.45
1:D:482:ARG:O	1:D:484:GLU:N	2.50	0.45
1:D:658:ARG:HG3	1:D:658:ARG:NH1	2.30	0.45
1:D:835:LEU:HD23	1:D:846:ILE:HG23	1.99	0.45
2:I:6:DA:H1'	2:I:7:DA:H5''	1.99	0.45
1:A:2:LYS:HE3	3:L:101:DG:O5'	2.17	0.44
1:A:140:ASP:OD1	1:A:140:ASP:C	2.60	0.44
1:B:167:ALA:O	1:B:178:VAL:HG12	2.17	0.44
1:B:171:GLN:C	1:B:173:GLN:H	2.25	0.44
1:B:188:TYR:HE2	1:B:190:PRO:HB3	1.80	0.44
1:B:700:GLY:HA3	1:B:710:LEU:HD23	1.98	0.44
1:B:810:THR:HG23	1:B:813:ARG:NH2	2.32	0.44
1:C:351:ALA:O	1:C:352:LYS:HB2	2.17	0.44
1:C:771:PHE:C	1:C:773:GLN:H	2.25	0.44
1:D:294:SER:C	1:D:296:PHE:N	2.73	0.44
1:D:647:TRP:HZ3	1:D:651:LEU:HD12	1.81	0.44
1:D:815:ILE:HD12	1:D:815:ILE:O	2.17	0.44
1:A:280:PHE:CD2	1:A:343:LEU:CD2	3.00	0.44
1:A:423:VAL:O	1:A:423:VAL:HG12	2.17	0.44
1:A:691:PRO:HD3	1:A:699:GLY:HA3	1.99	0.44
1:A:835:LEU:HD12	1:A:844:LYS:O	2.16	0.44
1:B:92:TYR:O	1:B:96:THR:HB	2.17	0.44
1:B:265:LEU:HD12	1:B:265:LEU:N	2.32	0.44
1:B:403:ARG:HA	1:B:701:PHE:HA	1.98	0.44
1:B:567:TYR:O	1:B:571:GLY:N	2.49	0.44
1:B:797:PRO:HG3	1:B:806:ARG:CZ	2.46	0.44
1:C:5:TYR:O	1:C:6:LEU:HD23	2.17	0.44
1:C:81:GLU:HB3	4:C:925:HOH:O	2.16	0.44
1:C:314:GLU:O	1:C:315:SER:C	2.60	0.44
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.90	0.44
1:D:109:ARG:NH2	1:D:208:LYS:CB	2.76	0.44
1:D:128:GLN:HE21	1:D:128:GLN:HB3	1.59	0.44
1:D:535:ALA:HA	1:D:538:LEU:HB2	1.98	0.44
3:J:110:DA:H2''	3:J:111:DT:H5''	1.99	0.44
1:A:249:ARG:HB3	1:A:264:THR:HB	2.00	0.44
1:A:506:PRO:HB2	1:A:535:ALA:HB2	1.99	0.44
1:A:775:ASN:O	1:A:776:TYR:C	2.60	0.44
1:B:250:VAL:HG23	1:B:250:VAL:O	2.16	0.44
1:B:776:TYR:OH	1:B:853:GLU:HB3	2.18	0.44
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.51	0.44
1:C:81:GLU:CD	1:C:384:ARG:NH2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:HB	1:D:97:TYR:CD1	2.53	0.44
1:D:171:GLN:CD	1:D:303:LEU:HD11	2.42	0.44
1:D:728:MET:SD	3:L:113:DC:H5'	2.57	0.44
2:G:10:DA:H2''	2:G:11:DC:H5'	1.97	0.44
1:A:152:LEU:O	1:A:158:ASN:HA	2.17	0.44
1:A:744:ALA:O	1:A:745:LEU:C	2.60	0.44
1:B:126:PRO:HG3	1:B:221:PHE:CD1	2.50	0.44
1:B:252:VAL:O	1:B:253:ILE:C	2.59	0.44
1:B:466:ASP:OD2	1:B:466:ASP:C	2.61	0.44
1:C:239:ALA:C	1:C:241:ARG:H	2.26	0.44
1:C:255:ASN:HD22	1:C:255:ASN:HA	1.58	0.44
1:D:475:ILE:O	1:D:479:PHE:HB2	2.16	0.44
1:D:597:ILE:CD1	1:D:663:ILE:HG23	2.44	0.44
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.53	0.44
1:B:553:MET:C	1:B:557:ILE:HG12	2.42	0.44
1:C:819:ILE:O	1:C:819:ILE:HG23	2.17	0.44
1:D:3:GLU:HB3	1:D:99:TYR:OH	2.16	0.44
1:D:359:PHE:O	1:D:361:PRO:HD3	2.18	0.44
1:D:660:GLU:CB	1:D:661:PRO:HD3	2.47	0.44
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.99	0.44
1:D:710:LEU:HD12	1:D:726:LYS:HB3	1.99	0.44
1:A:280:PHE:N	1:A:280:PHE:HD1	2.14	0.44
1:A:397:LYS:O	1:A:399:PRO:HD3	2.17	0.44
1:A:478:VAL:HG13	1:A:559:ARG:HD2	1.98	0.44
1:B:181:GLU:CD	1:B:181:GLU:H	2.24	0.44
1:B:358:VAL:C	1:B:360:SER:H	2.25	0.44
1:D:88:PHE:O	1:D:89:LYS:C	2.60	0.44
1:D:91:ALA:HA	1:D:370:PHE:HE1	1.83	0.44
1:D:252:VAL:HG23	1:D:252:VAL:O	2.18	0.44
1:D:406:TYR:HE2	1:D:647:TRP:CZ2	2.36	0.44
1:D:510:VAL:O	1:D:532:LYS:O	2.36	0.44
1:D:599:ARG:NH2	1:D:600:LYS:HE2	2.33	0.44
1:A:8:VAL:O	1:A:354:GLN:NE2	2.47	0.44
1:A:145:ARG:HB2	1:A:147:TYR:CE1	2.52	0.44
1:A:526:ILE:O	1:A:526:ILE:HG22	2.18	0.44
1:A:542:LEU:O	1:A:546:GLN:HG3	2.18	0.44
1:B:110:VAL:H	1:B:141:SER:CB	2.31	0.44
1:B:483:LYS:HZ2	1:B:483:LYS:HB2	1.83	0.44
1:B:534:SER:CB	1:B:537:SER:HB2	2.48	0.44
1:B:597:ILE:HD12	1:B:683:MET:HE1	2.00	0.44
1:B:606:ASN:HD21	1:B:613:GLY:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:TYR:O	1:C:99:TYR:N	2.50	0.44
1:C:147:TYR:N	1:C:147:TYR:CD1	2.85	0.44
1:D:216:TRP:CZ3	1:D:290:LEU:N	2.86	0.44
1:D:483:LYS:HG2	1:D:483:LYS:O	2.18	0.44
1:D:485:HIS:HB3	1:D:556:GLN:HB3	1.99	0.44
3:J:104:DG:H2"	3:J:105:DC:C6	2.52	0.44
1:A:410:PHE:N	1:A:410:PHE:HD1	2.16	0.44
1:A:685:ARG:HH21	1:A:717:GLY:N	2.15	0.44
1:B:166:ILE:HG22	1:B:175:GLY:HA2	2.00	0.44
1:B:775:ASN:ND2	1:B:777:ILE:HB	2.27	0.44
1:C:124:PRO:HB2	1:C:225:TYR:CE2	2.52	0.44
1:C:495:ASN:HB3	1:C:522:PHE:CE2	2.52	0.44
1:C:878:LYS:HB3	1:C:879:PRO:HD3	2.00	0.44
1:D:112:ASN:HB2	1:D:214:THR:C	2.43	0.44
1:D:119:SER:HA	1:D:120:PRO:HD3	1.80	0.44
1:D:496:GLY:HA2	1:D:499:ILE:CD1	2.47	0.44
1:A:402:ASN:HA	1:A:886:ALA:O	2.18	0.44
1:A:797:PRO:HB3	1:A:806:ARG:HG3	2.00	0.44
1:A:804:HIS:NE2	3:F:110:DA:OP1	2.38	0.44
1:A:833:LEU:HD22	1:A:866:MET:HE1	2.00	0.44
1:A:846:ILE:HD11	1:A:854:ILE:HD11	2.00	0.44
1:B:25:ARG:HG2	1:B:25:ARG:NH1	2.31	0.44
1:B:198:LEU:O	1:B:199:MET:C	2.60	0.44
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.53	0.44
1:B:475:ILE:HD13	1:B:475:ILE:O	2.18	0.44
1:B:700:GLY:HA2	1:B:753:LEU:CD2	2.44	0.44
1:C:343:LEU:CD1	1:C:558:ASN:ND2	2.81	0.44
1:C:578:TYR:CD1	1:C:578:TYR:C	2.95	0.44
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.65	0.44
1:D:241:ARG:C	1:D:243:SER:N	2.76	0.44
1:A:514:LEU:HD22	1:A:529:LYS:HE2	1.99	0.43
1:A:811:TYR:OH	1:A:815:ILE:HD13	2.18	0.43
1:B:115:ILE:HD11	1:B:221:PHE:CD2	2.53	0.43
1:B:143:ASP:O	1:B:144:ASP:HB3	2.18	0.43
1:C:13:ASP:CG	1:C:64:ASN:HB2	2.43	0.43
1:C:475:ILE:CG2	1:C:476:THR:N	2.79	0.43
1:C:761:GLN:HE22	1:C:893:LYS:HA	1.82	0.43
1:C:840:PRO:HD2	1:C:865:TRP:CD1	2.53	0.43
1:D:155:PRO:C	1:D:156:TYR:HD2	2.26	0.43
1:A:37:LEU:C	1:A:38:PHE:CD1	2.96	0.43
1:A:105:HIS:ND1	1:A:105:HIS:C	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:O	1:B:428:GLU:HG3	2.18	0.43
1:B:96:THR:HG22	1:B:96:THR:O	2.18	0.43
1:B:199:MET:HA	1:B:199:MET:HE3	2.00	0.43
1:B:365:TRP:CE2	1:B:566:LEU:HD13	2.53	0.43
1:B:773:GLN:CD	1:B:773:GLN:N	2.75	0.43
1:C:7:THR:CG2	1:C:211:VAL:HG13	2.48	0.43
1:C:606:ASN:OD1	1:C:614:GLU:HB2	2.18	0.43
1:C:839:ASN:HB2	1:C:840:PRO:HD2	2.00	0.43
1:D:50:PHE:N	1:D:50:PHE:CD1	2.87	0.43
1:D:428:GLU:OE1	1:D:469:GLY:HA2	2.18	0.43
1:D:779:ILE:HD13	1:D:780:ALA:N	2.33	0.43
1:A:159:VAL:HG21	1:A:317:HIS:CG	2.53	0.43
1:A:240:LYS:O	1:A:246:ARG:HA	2.18	0.43
1:A:629:ALA:O	1:A:630:ASP:C	2.60	0.43
1:A:782:VAL:O	1:A:783:SER:HB2	2.17	0.43
1:A:811:TYR:HH	1:A:822:PRO:C	2.26	0.43
1:A:831:TYR:N	1:A:848:TRP:O	2.51	0.43
1:A:871:LEU:O	1:A:875:THR:OG1	2.34	0.43
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.99	0.43
1:B:517:ASP:OD1	1:B:519:ARG:CB	2.64	0.43
1:B:685:ARG:HH11	1:B:685:ARG:CG	2.32	0.43
1:B:744:ALA:O	1:B:747:GLU:HB3	2.19	0.43
1:C:151:LEU:HD11	1:C:153:ASN:O	2.18	0.43
1:D:33:TYR:CE2	1:D:35:PRO:HA	2.52	0.43
1:D:317:HIS:CE1	1:D:321:ILE:HD13	2.53	0.43
1:D:326:ILE:HG22	1:D:330:ARG:HE	1.82	0.43
1:D:531:LYS:O	1:D:532:LYS:C	2.62	0.43
1:A:2:LYS:HA	1:A:2:LYS:CE	2.48	0.43
1:A:431:ALA:N	1:A:462:MET:O	2.44	0.43
1:A:643:ASP:CA	1:A:693:LEU:HD23	2.48	0.43
1:A:702:TRP:NE1	1:A:708:TYR:CD1	2.86	0.43
1:A:741:VAL:HG11	1:A:875:THR:O	2.19	0.43
1:A:869:THR:O	1:A:873:GLU:HB2	2.18	0.43
1:B:150:ASP:HB3	1:B:188:TYR:CE1	2.53	0.43
1:B:704:GLY:O	1:B:705:LYS:C	2.59	0.43
1:B:771:PHE:CD1	1:B:774:LEU:HD12	2.52	0.43
1:D:236:GLU:O	1:D:240:LYS:HG2	2.18	0.43
1:D:285:GLN:HE21	1:D:285:GLN:N	2.15	0.43
1:D:709:ALA:HB2	1:D:730:LEU:HD11	1.99	0.43
1:D:771:PHE:CE2	1:D:872:LEU:HB2	2.53	0.43
1:A:6:LEU:HG	1:A:19:TYR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLU:CD	1:B:181:GLU:N	2.76	0.43
1:B:233:ILE:N	1:B:233:ILE:CD1	2.82	0.43
1:B:530:ILE:C	1:B:532:LYS:N	2.76	0.43
1:C:607:GLU:O	1:C:609:CYS:N	2.52	0.43
1:C:898:PHE:CD2	1:C:898:PHE:N	2.85	0.43
1:D:212:ILE:CD1	1:D:345:LEU:HD21	2.43	0.43
1:D:416:TYR:O	1:D:417:PRO:C	2.61	0.43
1:D:839:ASN:ND2	1:D:839:ASN:O	2.51	0.43
1:A:5:TYR:HA	1:A:19:TYR:CB	2.49	0.43
1:A:745:LEU:CD1	1:A:876:PHE:CD1	3.01	0.43
1:A:775:ASN:O	1:A:778:SER:N	2.44	0.43
1:A:825:VAL:HG22	1:A:826:GLU:N	2.33	0.43
1:B:396:VAL:HB	2:G:7:DA:OP1	2.19	0.43
1:C:164:ILE:HG13	1:C:183:ILE:HD11	2.01	0.43
1:C:239:ALA:C	1:C:241:ARG:N	2.77	0.43
1:C:271:LEU:HD21	1:C:356:GLN:HA	2.01	0.43
1:D:113:PHE:CE1	1:D:218:VAL:HG13	2.54	0.43
1:D:253:ILE:O	1:D:253:ILE:HG13	2.18	0.43
1:D:493:GLN:CG	1:D:494:ARG:H	2.14	0.43
1:A:109:ARG:HD2	1:A:209:THR:O	2.19	0.43
1:A:279:LYS:HB3	1:A:280:PHE:CE1	2.54	0.43
1:A:389:GLN:HE21	1:A:389:GLN:HB3	1.54	0.43
1:A:529:LYS:HB3	1:A:529:LYS:NZ	2.34	0.43
1:B:140:ASP:C	1:B:140:ASP:OD1	2.61	0.43
1:B:177:GLU:O	1:B:178:VAL:C	2.61	0.43
1:B:330:ARG:O	1:B:334:ILE:HG13	2.19	0.43
1:C:202:LEU:CD2	1:C:241:ARG:HH21	2.31	0.43
1:C:458:PRO:HG2	1:C:592:MET:SD	2.59	0.43
1:C:474:GLU:OE2	1:C:477:LYS:NZ	2.52	0.43
1:C:579:ASP:O	1:C:580:LEU:C	2.62	0.43
1:D:133:ILE:HG12	1:D:229:ARG:CD	2.38	0.43
1:D:491:ALA:HB1	1:D:521:ASP:OD1	2.18	0.43
1:D:687:ALA:HA	1:D:714:ASP:O	2.19	0.43
2:G:15:DC:H2'	2:G:16:DG:C8	2.53	0.43
1:A:548:THR:O	1:A:549:GLU:C	2.61	0.43
1:A:835:LEU:O	1:A:837:GLU:N	2.52	0.43
1:B:130:LYS:NZ	1:B:130:LYS:CB	2.81	0.43
1:B:211:VAL:O	1:B:211:VAL:HG12	2.17	0.43
1:B:443:ILE:HD13	1:B:595:GLN:HB3	2.00	0.43
1:B:446:VAL:O	1:B:446:VAL:CG2	2.60	0.43
1:C:251:LYS:O	1:C:261:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:GLY:O	1:C:500:LYS:HG3	2.18	0.43
1:C:702:TRP:CZ3	1:C:710:LEU:HD21	2.53	0.43
1:D:109:ARG:NH2	1:D:140:ASP:OD2	2.52	0.43
1:D:292:TYR:C	1:D:292:TYR:CD1	2.97	0.43
3:F:110:DA:C2'	3:F:111:DT:C5'	2.94	0.43
1:A:779:ILE:O	1:A:871:LEU:HD21	2.18	0.43
1:B:727:ILE:HG23	1:B:730:LEU:HD12	2.01	0.43
1:C:133:ILE:HG13	1:C:229:ARG:HG2	2.01	0.43
1:D:19:TYR:N	1:D:19:TYR:CD1	2.86	0.43
1:D:62:PHE:HZ	1:D:71:TRP:CE3	2.37	0.43
1:D:132:PRO:CA	1:D:229:ARG:NH2	2.79	0.43
1:D:230:ILE:CG2	1:D:239:ALA:HA	2.49	0.43
1:D:417:PRO:O	1:D:420:ILE:N	2.52	0.43
1:A:87:ASP:CG	1:A:90:LEU:HG	2.44	0.43
1:A:120:PRO:HG2	1:A:156:TYR:HE1	1.81	0.43
1:B:135:ALA:HB1	1:B:324:ASN:HD22	1.84	0.43
1:B:170:LEU:N	1:B:170:LEU:CD1	2.82	0.43
1:B:186:ILE:O	1:B:187:ILE:CG1	2.67	0.43
1:B:412:LEU:HB2	1:B:623:ASP:HB2	2.01	0.43
1:B:441:ASP:HB3	1:B:447:ALA:HB2	2.00	0.43
1:B:555:ALA:O	1:B:559:ARG:HD3	2.18	0.43
1:B:880:LEU:O	1:B:884:THR:HG23	2.19	0.43
1:C:154:SER:OG	1:C:313:ARG:NH2	2.52	0.43
1:C:271:LEU:HB3	1:C:276:LEU:HD21	2.00	0.43
1:C:836:ARG:NH1	1:C:836:ARG:HG3	2.34	0.43
1:D:73:LYS:O	1:D:77:ASP:OD2	2.36	0.43
1:D:573:VAL:HA	1:D:578:TYR:CD2	2.54	0.43
1:D:825:VAL:HB	1:D:828:GLU:HG3	2.00	0.43
3:H:105:DC:C2'	3:H:106:DT:H71	2.49	0.43
1:A:45:GLN:O	1:A:47:THR:HG23	2.18	0.42
1:A:85:MET:HE1	1:A:366:ASP:OD2	2.18	0.42
1:A:294:SER:O	1:A:298:LEU:HD12	2.19	0.42
1:A:299:ASN:O	1:A:300:VAL:HB	2.18	0.42
1:B:145:ARG:HG2	1:B:187:ILE:CD1	2.48	0.42
1:B:186:ILE:CG2	1:B:187:ILE:H	2.32	0.42
1:B:214:THR:OG1	1:B:273:TYR:HD2	2.02	0.42
1:B:331:VAL:O	1:B:334:ILE:HB	2.19	0.42
1:C:461:MET:SD	1:C:581:ARG:HB3	2.59	0.42
1:C:681:MET:HE2	1:C:681:MET:HA	2.00	0.42
1:C:706:LYS:C	1:C:707:ARG:HG2	2.43	0.42
1:D:125:GLU:HG3	1:D:127:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:803:PHE:O	1:D:806:ARG:HB2	2.19	0.42
1:A:656:ARG:HA	1:A:660:GLU:CG	2.48	0.42
1:A:745:LEU:O	1:A:749:ILE:HG13	2.19	0.42
1:B:76:GLU:OE1	1:B:382:GLN:NE2	2.52	0.42
1:B:597:ILE:CD1	1:B:683:MET:SD	3.07	0.42
1:B:685:ARG:CZ	1:B:688:ILE:HD11	2.48	0.42
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.34	0.42
1:C:323:TYR:O	1:C:326:ILE:N	2.52	0.42
1:C:453:VAL:CG2	1:C:454:TYR:N	2.82	0.42
1:D:513:PRO:HA	1:D:541:MET:HE1	2.01	0.42
1:D:573:VAL:C	1:D:575:PHE:N	2.77	0.42
1:D:597:ILE:CG2	1:D:598:GLU:N	2.82	0.42
1:A:120:PRO:CG	1:A:156:TYR:CE1	3.02	0.42
1:A:502:ALA:O	1:A:503:LEU:HD12	2.19	0.42
1:A:621:ASP:HB3	3:F:114:DA:C5'	2.50	0.42
1:A:737:THR:O	1:A:738:PRO:C	2.60	0.42
1:B:120:PRO:HG2	1:B:156:TYR:HE2	1.82	0.42
1:B:154:SER:C	1:B:156:TYR:H	2.27	0.42
1:B:840:PRO:HD3	1:B:865:TRP:CE2	2.55	0.42
1:C:9:GLU:HG3	1:C:267:GLY:H	1.85	0.42
1:C:254:GLU:HG2	1:C:259:SER:HB2	2.01	0.42
1:C:319:ARG:O	1:C:320:TYR:C	2.61	0.42
1:C:321:ILE:O	1:C:325:ILE:HG13	2.19	0.42
1:C:360:SER:O	1:C:361:PRO:C	2.61	0.42
1:C:474:GLU:O	1:C:475:ILE:C	2.62	0.42
1:C:503:LEU:HG	1:C:538:LEU:HB3	2.01	0.42
1:D:105:HIS:ND1	1:D:106:THR:N	2.67	0.42
1:D:180:SER:C	1:D:182:ILE:N	2.75	0.42
1:D:369:ILE:O	1:D:370:PHE:C	2.62	0.42
1:D:456:CYS:HB3	1:D:461:MET:O	2.19	0.42
1:D:484:GLU:OE1	1:D:485:HIS:ND1	2.43	0.42
1:D:726:LYS:HE3	1:D:728:MET:HE3	2.02	0.42
2:E:15:DC:H2''	2:E:16:DG:C8	2.54	0.42
2:G:6:DA:C2'	2:G:7:DA:H5''	2.49	0.42
2:G:10:DA:C2'	2:G:11:DC:H5''	2.48	0.42
2:K:7:DA:H2''	2:K:8:DT:OP2	2.20	0.42
1:A:83:LEU:N	1:A:83:LEU:CD1	2.82	0.42
1:A:397:LYS:HD3	1:A:619:TYR:HA	2.00	0.42
1:A:625:ILE:HG12	1:A:683:MET:HE1	2.00	0.42
1:A:811:TYR:OH	1:A:822:PRO:C	2.63	0.42
1:B:422:GLN:HG2	1:B:676:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:NH1	1:C:208:LYS:CD	2.79	0.42
1:C:128:GLN:HE21	1:C:128:GLN:HB3	1.61	0.42
1:C:264:THR:O	1:C:265:LEU:HD23	2.20	0.42
1:C:722:GLU:OE1	1:C:722:GLU:HA	2.20	0.42
1:D:88:PHE:C	1:D:90:LEU:N	2.77	0.42
1:D:244:PRO:O	1:D:245:HIS:HD2	2.02	0.42
1:D:342:ASN:O	1:D:343:LEU:C	2.63	0.42
1:D:391:TYR:HB2	1:D:392:PRO:CD	2.42	0.42
1:D:655:ALA:HA	1:D:659:MET:HB2	2.01	0.42
1:D:870:VAL:O	1:D:874:LYS:HG2	2.19	0.42
2:I:3:DT:H5'	2:I:3:DT:C6	2.55	0.42
2:K:8:DT:C2'	2:K:9:DG:C8	3.03	0.42
1:A:51:ASP:OD1	1:A:51:ASP:C	2.62	0.42
1:A:206:GLN:OE1	1:A:241:ARG:HB3	2.19	0.42
1:A:410:PHE:CB	1:A:683:MET:HE2	2.50	0.42
1:A:434:PHE:O	1:A:435:LYS:C	2.62	0.42
1:B:442:TYR:O	1:B:596:TRP:HZ3	2.02	0.42
1:B:757:GLU:O	1:B:761:GLN:HG3	2.19	0.42
1:C:97:TYR:HA	1:C:99:TYR:CE1	2.54	0.42
1:C:143:ASP:O	1:C:144:ASP:CB	2.67	0.42
1:C:635:LYS:HD2	1:C:635:LYS:O	2.19	0.42
1:D:33:TYR:OH	1:D:95:ASP:OD2	2.31	0.42
1:D:616:PHE:O	1:D:627:VAL:HA	2.19	0.42
1:A:2:LYS:NZ	1:A:2:LYS:CA	2.74	0.42
1:A:154:SER:O	1:A:155:PRO:C	2.61	0.42
1:A:410:PHE:HA	1:A:684:ASP:O	2.20	0.42
1:B:273:TYR:O	1:B:277:TYR:HB2	2.20	0.42
1:B:425:ILE:HG23	1:B:463:TYR:CZ	2.54	0.42
1:B:831:TYR:CD2	1:B:850:SER:HA	2.55	0.42
1:B:841:PHE:CE2	1:B:862:VAL:HG22	2.54	0.42
1:C:28:THR:O	1:C:28:THR:CG2	2.67	0.42
1:C:249:ARG:HB3	1:C:264:THR:HB	2.02	0.42
1:C:249:ARG:O	1:C:263:ILE:HA	2.20	0.42
1:C:285:GLN:O	1:C:829:LYS:NZ	2.45	0.42
1:C:570:LEU:HD23	1:C:575:PHE:HE2	1.84	0.42
1:D:535:ALA:HB1	1:D:539:ASN:HD21	1.82	0.42
1:D:561:LEU:HD23	1:D:561:LEU:C	2.44	0.42
1:A:50:PHE:CD2	1:A:56:PRO:HA	2.54	0.42
1:A:140:ASP:OD1	1:A:142:ILE:N	2.53	0.42
1:A:621:ASP:CG	3:F:114:DA:H5'	2.44	0.42
1:A:737:THR:C	1:A:738:PRO:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:VAL:HG13	1:A:849:PRO:CG	2.47	0.42
1:B:659:MET:O	1:B:660:GLU:C	2.61	0.42
1:C:147:TYR:CB	1:C:149:PHE:HE1	2.30	0.42
1:D:493:GLN:HB3	1:D:549:GLU:HG3	2.02	0.42
1:A:150:ASP:OD1	1:A:317:HIS:NE2	2.52	0.42
1:A:277:TYR:HA	1:A:340:PHE:CE2	2.55	0.42
1:A:384:ARG:HG3	1:A:386:HIS:CE1	2.54	0.42
1:A:606:ASN:ND2	1:A:613:GLY:HA2	2.35	0.42
1:A:861:ASP:OD2	1:A:861:ASP:N	2.52	0.42
1:B:96:THR:HG22	1:B:97:TYR:CD2	2.55	0.42
1:B:125:GLU:HA	1:B:126:PRO:HD3	1.90	0.42
1:B:604:TYR:O	1:B:607:GLU:HB3	2.20	0.42
1:B:702:TRP:CZ2	1:B:708:TYR:CD2	3.08	0.42
1:B:773:GLN:H	1:B:773:GLN:CD	2.27	0.42
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.55	0.42
1:C:680:LEU:C	1:C:681:MET:HE2	2.44	0.42
1:C:806:ARG:O	1:C:807:GLY:C	2.62	0.42
1:D:101:ILE:O	1:D:102:LYS:HE3	2.20	0.42
1:D:234:PHE:N	1:D:234:PHE:CD1	2.87	0.42
1:D:376:GLN:O	1:D:377:ASN:C	2.62	0.42
1:D:526:ILE:HG13	1:D:526:ILE:O	2.19	0.42
1:A:82:ALA:O	1:A:382:GLN:HB2	2.20	0.42
1:A:171:GLN:HE22	1:A:319:ARG:NH1	2.10	0.42
1:A:734:LYS:HB3	1:A:737:THR:OG1	2.20	0.42
1:A:736:SER:HB2	1:A:782:VAL:O	2.20	0.42
1:A:799:PRO:HD2	4:A:920:HOH:O	2.19	0.42
1:B:3:GLU:HG2	1:B:21:ASP:C	2.45	0.42
1:B:151:LEU:HG	1:B:153:ASN:O	2.20	0.42
1:B:374:LYS:O	1:B:376:GLN:N	2.52	0.42
1:B:472:PRO:HA	1:B:475:ILE:HG22	2.01	0.42
1:B:678:GLN:HG2	1:B:680:LEU:HG	2.01	0.42
1:B:761:GLN:OE1	1:B:893:LYS:HE3	2.19	0.42
1:C:149:PHE:CD1	1:C:149:PHE:N	2.86	0.42
1:C:400:ILE:O	1:C:401:PRO:C	2.63	0.42
1:C:457:SER:HA	1:C:458:PRO:HD3	1.86	0.42
1:C:482:ARG:NH1	1:C:556:GLN:HG2	2.35	0.42
1:C:692:PRO:HD2	1:C:695:SER:OG	2.19	0.42
1:C:774:LEU:O	1:C:775:ASN:C	2.63	0.42
1:D:147:TYR:N	1:D:147:TYR:CD1	2.87	0.42
1:D:584:THR:O	1:D:585:ALA:C	2.60	0.42
1:D:839:ASN:ND2	1:D:839:ASN:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:839:ASN:OD1	1:D:843:ASP:O	2.38	0.42
3:H:110:DA:C2'	3:H:111:DT:H5''	2.50	0.42
1:A:159:VAL:HG23	1:A:160:GLU:O	2.20	0.42
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.84	0.42
1:A:415:LEU:O	1:A:419:ILE:HG13	2.20	0.42
1:A:621:ASP:HB3	3:F:114:DA:H5''	2.02	0.42
1:A:766:GLU:C	1:A:768:GLU:N	2.78	0.42
1:B:362:ILE:CD1	1:B:575:PHE:HB2	2.50	0.42
1:B:499:ILE:HG13	1:B:542:LEU:HD13	2.02	0.42
1:B:559:ARG:O	1:B:563:ILE:HG13	2.19	0.42
1:B:706:LYS:HE2	3:H:113:DC:O2	2.20	0.42
1:C:254:GLU:HG2	1:C:259:SER:CB	2.50	0.42
1:D:771:PHE:CD2	1:D:872:LEU:HD13	2.55	0.42
1:A:389:GLN:HA	1:A:390:PRO:HD3	1.83	0.41
1:A:602:ASN:ND2	1:A:616:PHE:H	2.18	0.41
1:A:792:ASP:CG	1:A:792:ASP:O	2.60	0.41
1:B:13:ASP:OD2	1:B:66:ARG:HB2	2.20	0.41
1:B:104:ASP:OD2	1:B:106:THR:OG1	2.38	0.41
1:B:116:GLU:OE1	1:B:116:GLU:HA	2.19	0.41
1:B:312:LEU:HD12	1:B:320:TYR:CD1	2.55	0.41
1:B:901:PHE:HB3	1:D:608:VAL:CG1	2.50	0.41
1:C:81:GLU:CD	1:C:384:ARG:HH21	2.28	0.41
1:C:292:TYR:O	1:C:295:GLU:HB3	2.19	0.41
1:C:524:ASP:HA	1:C:527:LYS:HE3	2.01	0.41
1:D:423:VAL:HB	1:D:425:ILE:HG13	2.00	0.41
3:J:112:DT:H2'	3:J:113:DC:C5	2.55	0.41
1:A:408:MET:HE3	1:A:688:ILE:HD11	2.01	0.41
1:A:514:LEU:HD21	1:A:529:LYS:HE2	2.01	0.41
1:A:516:VAL:CG1	1:A:526:ILE:HG13	2.50	0.41
1:A:618:LEU:HG	1:A:619:TYR:N	2.34	0.41
1:A:839:ASN:HB3	1:A:865:TRP:CE3	2.55	0.41
1:B:248:THR:CG2	1:B:265:LEU:HA	2.44	0.41
1:B:463:TYR:CD1	1:B:463:TYR:N	2.88	0.41
1:B:621:ASP:O	1:B:623:ASP:N	2.51	0.41
1:B:894:LYS:HB2	1:B:894:LYS:HZ3	1.78	0.41
1:C:256:MET:HB3	1:C:257:TYR:CD1	2.55	0.41
1:C:261:GLU:H	1:C:261:GLU:HG2	1.74	0.41
1:C:469:GLY:C	1:C:472:PRO:HD2	2.44	0.41
1:D:131:HIS:HB2	1:D:225:TYR:OH	2.20	0.41
1:D:329:TYR:CE2	1:D:333:GLN:CD	2.98	0.41
1:D:686:GLU:OE1	1:D:686:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DA:C2'	2:E:7:DA:C5'	2.84	0.41
1:A:104:ASP:C	1:A:106:THR:N	2.78	0.41
1:A:800:LYS:O	1:A:802:PRO:HD3	2.21	0.41
1:B:61:LEU:HD23	1:B:62:PHE:H	1.85	0.41
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.78	0.41
1:B:132:PRO:HB3	1:B:194:GLU:OE2	2.20	0.41
1:C:32:GLU:OE1	1:C:32:GLU:HA	2.20	0.41
1:C:303:LEU:HB3	1:C:319:ARG:HH11	1.85	0.41
1:D:129:ALA:HB1	1:D:225:TYR:CE2	2.55	0.41
1:D:478:VAL:HG11	1:D:562:LEU:HD22	2.03	0.41
1:D:496:GLY:HA2	1:D:499:ILE:HD12	2.03	0.41
3:L:108:DT:H2''	3:L:109:DC:O5'	2.21	0.41
1:A:6:LEU:HD13	1:A:211:VAL:HG21	2.01	0.41
1:A:279:LYS:HE2	1:A:359:PHE:HA	2.00	0.41
1:A:654:PHE:CD1	1:A:654:PHE:C	2.97	0.41
1:A:776:TYR:CE2	1:A:777:ILE:HG13	2.56	0.41
1:A:776:TYR:CG	1:A:863:LEU:HD11	2.55	0.41
1:A:809:LEU:HD23	1:A:812:ASN:ND2	2.36	0.41
1:B:193:ASN:HB3	1:B:196:GLU:CG	2.50	0.41
1:B:834:PRO:O	1:B:867:ASP:N	2.50	0.41
1:C:33:TYR:OH	1:C:95:ASP:OD1	2.32	0.41
1:C:73:LYS:O	1:C:74:ARG:C	2.64	0.41
1:C:558:ASN:HD22	1:C:558:ASN:HA	1.65	0.41
1:C:811:TYR:CA	1:C:846:ILE:HD11	2.50	0.41
1:D:91:ALA:O	1:D:94:SER:HB2	2.19	0.41
1:D:218:VAL:HG12	1:D:223:ILE:CD1	2.50	0.41
1:D:421:ARG:CD	1:D:475:ILE:HG23	2.51	0.41
2:E:16:DG:N2	3:F:103:DG:C2	2.89	0.41
1:A:61:LEU:C	1:A:61:LEU:CD2	2.93	0.41
1:A:334:ILE:O	1:A:337:LYS:HB2	2.20	0.41
1:A:471:VAL:HB	1:A:472:PRO:HD3	2.01	0.41
1:A:725:LEU:HD12	1:A:746:LYS:HE2	2.02	0.41
1:B:197:LEU:C	1:B:197:LEU:CD2	2.94	0.41
1:B:209:THR:HA	1:B:210:PRO:HD3	1.80	0.41
1:B:280:PHE:CD1	1:B:280:PHE:N	2.88	0.41
1:B:416:TYR:HB2	1:B:417:PRO:HD3	2.02	0.41
1:B:546:GLN:O	1:B:550:VAL:HG23	2.21	0.41
1:C:147:TYR:N	1:C:147:TYR:HD1	2.17	0.41
1:C:561:LEU:HD12	1:C:561:LEU:HA	1.82	0.41
1:C:577:TYR:CD2	1:C:577:TYR:N	2.88	0.41
1:C:731:GLU:OE2	1:C:879:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ARG:HH21	1:D:211:VAL:HG22	1.84	0.41
1:D:82:ALA:H	1:D:382:GLN:CG	2.33	0.41
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.55	0.41
1:D:305:TYR:CD2	1:D:305:TYR:C	2.98	0.41
1:D:533:LEU:HB3	1:D:537:SER:OG	2.20	0.41
1:D:825:VAL:HG12	1:D:826:GLU:H	1.86	0.41
1:D:890:ASP:N	1:D:890:ASP:OD2	2.51	0.41
1:A:396:VAL:HG21	1:A:706:LYS:NZ	2.35	0.41
1:A:467:ARG:HD3	1:A:467:ARG:H	1.85	0.41
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.51	0.41
1:B:85:MET:HA	1:B:380:ILE:HD11	2.03	0.41
1:B:476:THR:O	1:B:477:LYS:C	2.63	0.41
1:B:727:ILE:HB	1:B:733:GLN:NE2	2.36	0.41
1:B:783:SER:O	1:B:829:LYS:HA	2.20	0.41
1:C:97:TYR:CD1	1:C:97:TYR:N	2.89	0.41
1:C:140:ASP:OD1	1:C:142:ILE:HB	2.21	0.41
1:C:189:MET:O	1:C:191:PHE:CD1	2.74	0.41
1:C:221:PHE:C	1:C:224:PRO:HD2	2.46	0.41
1:C:420:ILE:HG21	1:C:471:VAL:HG12	2.03	0.41
1:C:493:GLN:HA	1:C:549:GLU:OE2	2.21	0.41
1:C:761:GLN:NE2	1:C:893:LYS:HA	2.36	0.41
1:D:416:TYR:HD2	1:D:586:ILE:HG22	1.85	0.41
1:D:425:ILE:O	1:D:426:SER:HB2	2.20	0.41
1:D:533:LEU:HD11	1:D:536:LYS:HB2	2.03	0.41
1:D:602:ASN:HD21	1:D:617:VAL:HG22	1.86	0.41
2:G:5:DG:H2''	2:G:6:DA:O5'	2.21	0.41
2:G:15:DC:H2''	2:G:16:DG:C5'	2.50	0.41
2:I:12:DA:H2''	2:I:13:DG:C5'	2.50	0.41
1:A:52:ILE:HD12	1:A:428:GLU:HB3	2.03	0.41
1:A:506:PRO:HB2	1:A:535:ALA:CA	2.50	0.41
1:B:488:TYR:C	1:B:490:LEU:N	2.77	0.41
1:B:837:GLU:HG2	1:B:838:GLY:H	1.82	0.41
1:C:111:ALA:HB2	1:C:210:PRO:HB3	2.01	0.41
1:C:162:TRP:HB3	1:C:188:TYR:CE2	2.55	0.41
1:C:516:VAL:HG21	1:C:522:PHE:HE1	1.82	0.41
1:C:738:PRO:HG2	1:C:741:VAL:HB	2.02	0.41
1:D:458:PRO:C	1:D:460:GLY:N	2.79	0.41
1:D:470:VAL:HG13	1:D:471:VAL:N	2.36	0.41
1:D:578:TYR:OH	1:D:580:LEU:HD13	2.21	0.41
1:D:685:ARG:HD2	1:D:685:ARG:O	2.21	0.41
1:A:175:GLY:O	1:A:319:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:O	1:A:186:ILE:HG13	2.21	0.41
1:A:231:LYS:O	1:A:235:GLY:N	2.44	0.41
1:A:602:ASN:HD21	1:A:616:PHE:N	2.18	0.41
1:A:660:GLU:HB2	1:A:661:PRO:CD	2.49	0.41
1:B:171:GLN:CD	1:B:303:LEU:HD13	2.46	0.41
1:C:558:ASN:O	1:C:559:ARG:C	2.61	0.41
1:C:757:GLU:O	1:C:761:GLN:HG3	2.20	0.41
1:D:2:LYS:CG	1:D:3:GLU:H	2.33	0.41
1:D:170:LEU:HD22	1:D:177:GLU:OE2	2.20	0.41
1:D:216:TRP:O	1:D:217:ASN:HB2	2.21	0.41
1:D:321:ILE:N	1:D:321:ILE:CD1	2.83	0.41
1:D:373:LEU:O	1:D:378:LYS:HB2	2.20	0.41
1:D:560:LYS:O	1:D:561:LEU:C	2.63	0.41
1:A:119:SER:HA	1:A:120:PRO:HD3	1.93	0.41
1:B:202:LEU:HD11	1:B:241:ARG:HB3	2.02	0.41
1:B:457:SER:HA	1:B:458:PRO:HD3	1.86	0.41
1:B:703:THR:OG1	1:B:704:GLY:N	2.53	0.41
1:C:92:TYR:CD1	1:C:92:TYR:C	2.98	0.41
1:C:253:ILE:O	1:C:259:SER:HA	2.21	0.41
1:C:257:TYR:CD1	1:C:257:TYR:N	2.89	0.41
1:C:789:ALA:O	1:C:790:LYS:C	2.64	0.41
1:D:271:LEU:HB3	1:D:276:LEU:HD21	2.03	0.41
1:D:345:LEU:O	1:D:346:ASP:C	2.63	0.41
1:D:367:ALA:O	1:D:370:PHE:HB3	2.21	0.41
1:D:421:ARG:HD2	1:D:476:THR:OG1	2.20	0.41
1:D:569:ALA:C	1:D:571:GLY:N	2.77	0.41
1:D:639:SER:C	1:D:641:PHE:N	2.79	0.41
2:G:13:DG:H2''	2:G:14:DC:O5'	2.20	0.41
3:J:112:DT:C2'	3:J:113:DC:C6	3.04	0.41
1:A:729:GLY:O	1:A:730:LEU:C	2.64	0.41
1:A:898:PHE:CD1	1:A:898:PHE:N	2.86	0.41
1:B:343:LEU:O	1:B:344:SER:C	2.64	0.41
1:B:469:GLY:O	1:B:472:PRO:HG2	2.20	0.41
1:B:771:PHE:O	1:B:774:LEU:HB2	2.20	0.41
1:B:776:TYR:CE2	1:B:854:ILE:HG22	2.56	0.41
1:B:791:TYR:HE2	1:B:800:LYS:O	2.04	0.41
1:B:810:THR:O	1:B:810:THR:HG22	2.21	0.41
1:C:256:MET:SD	1:C:257:TYR:CE1	3.14	0.41
1:C:271:LEU:HD11	1:C:355:ILE:HG22	2.02	0.41
1:C:543:PHE:O	1:C:547:ARG:HB2	2.21	0.41
1:C:659:MET:O	1:C:663:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PHE:N	1:D:62:PHE:CD1	2.89	0.41
1:D:883:PHE:N	1:D:883:PHE:HD2	2.18	0.41
2:E:7:DA:H2'	2:E:8:DT:H72	2.02	0.41
1:C:83:LEU:HD22	1:C:83:LEU:H	1.86	0.40
1:C:272:ASP:CG	1:C:274:ILE:HG22	2.46	0.40
1:C:518:TYR:CD1	1:C:518:TYR:N	2.89	0.40
1:D:171:GLN:HG2	1:D:319:ARG:HH22	1.85	0.40
1:D:216:TRP:HZ3	1:D:288:TYR:O	2.03	0.40
1:D:317:HIS:CE1	1:D:321:ILE:CD1	3.04	0.40
1:D:835:LEU:HD11	1:D:843:ASP:O	2.21	0.40
1:A:194:GLU:CD	1:A:229:ARG:HH11	2.26	0.40
1:A:197:LEU:O	1:A:198:LEU:C	2.64	0.40
1:A:280:PHE:HD2	1:A:343:LEU:HD21	1.84	0.40
1:A:480:ASN:O	1:A:481:GLN:C	2.64	0.40
1:A:550:VAL:O	1:A:551:ALA:C	2.64	0.40
1:A:618:LEU:HD23	1:A:626:TYR:O	2.21	0.40
1:A:685:ARG:NH1	1:A:685:ARG:HG2	2.37	0.40
1:B:137:THR:HG22	1:B:328:VAL:HG21	2.02	0.40
1:B:285:GLN:HG2	1:B:293:ILE:HD13	2.03	0.40
1:C:454:TYR:HD2	1:C:462:MET:HE3	1.84	0.40
1:C:484:GLU:HG2	1:C:488:TYR:CE2	2.56	0.40
1:C:540:GLU:HA	1:C:540:GLU:OE1	2.21	0.40
1:C:703:THR:HG22	1:C:886:ALA:CB	2.52	0.40
1:D:348:GLY:HA3	1:D:355:ILE:HD13	2.03	0.40
1:D:769:LYS:O	1:D:773:GLN:NE2	2.54	0.40
1:A:218:VAL:CG2	1:A:223:ILE:HG13	2.52	0.40
1:A:362:ILE:HG12	1:A:572:ASN:HD21	1.80	0.40
1:A:432:GLY:O	1:A:462:MET:N	2.55	0.40
1:A:553:MET:O	1:A:556:GLN:HG3	2.21	0.40
1:B:89:LYS:HE3	1:B:354:GLN:NE2	2.36	0.40
1:B:245:HIS:O	1:B:246:ARG:C	2.64	0.40
1:B:433:THR:HA	1:B:460:GLY:O	2.21	0.40
1:B:508:LEU:H	1:B:508:LEU:CD2	2.23	0.40
1:B:560:LYS:O	1:B:561:LEU:C	2.63	0.40
1:B:597:ILE:CD1	1:B:683:MET:HE1	2.51	0.40
1:B:735:SER:C	1:B:737:THR:N	2.79	0.40
1:C:253:ILE:HD13	2:I:1:DC:C5	2.56	0.40
1:D:358:VAL:O	1:D:358:VAL:HG12	2.20	0.40
1:D:597:ILE:HG12	1:D:683:MET:HE1	2.02	0.40
1:D:750:ARG:NH2	1:D:755:GLU:OE1	2.54	0.40
1:A:8:VAL:C	1:A:9:GLU:HG2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CE1	1:A:218:VAL:CG2	3.05	0.40
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.97	0.40
1:A:338:ARG:NH1	1:A:338:ARG:HG3	2.36	0.40
1:A:546:GLN:HA	1:A:549:GLU:HB2	2.03	0.40
1:A:805:ILE:C	1:A:807:GLY:H	2.28	0.40
1:A:846:ILE:HD12	1:A:846:ILE:C	2.46	0.40
1:B:223:ILE:HB	1:B:224:PRO:CD	2.44	0.40
1:B:626:TYR:CD1	1:B:626:TYR:N	2.89	0.40
1:C:273:TYR:CE2	1:C:335:ASP:HB2	2.57	0.40
1:C:537:SER:O	1:C:541:MET:HG3	2.22	0.40
1:C:582:ASN:O	1:C:585:ALA:HB3	2.21	0.40
1:C:742:GLN:O	1:C:743:LYS:C	2.65	0.40
1:C:880:LEU:O	1:C:881:GLU:C	2.63	0.40
1:D:456:CYS:HA	1:D:461:MET:O	2.21	0.40
1:D:458:PRO:HB2	1:D:588:THR:HG22	2.02	0.40
1:D:854:ILE:O	1:D:855:THR:C	2.63	0.40
3:F:106:DT:H1'	3:F:107:DG:C5'	2.44	0.40
3:H:110:DA:H1'	3:H:111:DT:H5''	2.02	0.40
1:A:193:ASN:HD21	1:A:196:GLU:CD	2.29	0.40
1:A:392:PRO:C	1:A:587:THR:HG21	2.44	0.40
1:A:410:PHE:HB2	1:A:683:MET:CE	2.51	0.40
1:B:117:VAL:HG11	1:B:225:TYR:OH	2.21	0.40
1:B:326:ILE:O	1:B:330:ARG:CG	2.66	0.40
1:B:355:ILE:HD13	1:B:355:ILE:HA	1.90	0.40
1:B:443:ILE:HD13	1:B:595:GLN:CB	2.51	0.40
1:B:520:PHE:O	1:B:521:ASP:C	2.64	0.40
1:B:837:GLU:CG	1:B:838:GLY:H	2.34	0.40
1:C:229:ARG:O	1:C:230:ILE:C	2.64	0.40
1:C:332:LEU:O	1:C:336:ALA:HB2	2.22	0.40
1:C:365:TRP:CD2	1:C:566:LEU:HD13	2.56	0.40
1:C:393:GLY:O	1:C:587:THR:HG23	2.22	0.40
1:C:503:LEU:HD21	1:C:538:LEU:HB2	2.03	0.40
1:C:514:LEU:CD2	1:C:526:ILE:HG23	2.51	0.40
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.96	0.40
1:D:61:LEU:HD23	1:D:61:LEU:C	2.45	0.40
1:D:302:LYS:N	1:D:302:LYS:HD2	2.37	0.40
1:D:318:GLN:O	1:D:322:SER:HB2	2.21	0.40
1:D:468:ASP:OD2	1:D:677:LYS:HE2	2.22	0.40
1:D:546:GLN:O	1:D:549:GLU:HB3	2.22	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%)	745 (83%)	129 (14%)	26 (3%)	3	20
1	B	900/906 (99%)	761 (85%)	119 (13%)	20 (2%)	5	26
1	C	899/906 (99%)	748 (83%)	125 (14%)	26 (3%)	3	20
1	D	886/906 (98%)	710 (80%)	133 (15%)	43 (5%)	1	10
All	All	3585/3624 (99%)	2964 (83%)	506 (14%)	115 (3%)	3	18

All (115) Ramachandran outliers are listed below:

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	789/803 (98%)	712 (90%)	77 (10%)	7	30
1	B	773/803 (96%)	715 (92%)	58 (8%)	12	41
1	C	794/803 (99%)	742 (94%)	52 (6%)	15	47
1	D	737/803 (92%)	677 (92%)	60 (8%)	11	38
All	All	3093/3212 (96%)	2846 (92%)	247 (8%)	11	38

All (247) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	86	ASP
1	A	94	SER
1	A	105	HIS
1	A	130	LYS
1	A	140	ASP
1	A	196	GLU
1	A	213	LEU
1	A	220	SER
1	A	229	ARG
1	A	231	LYS
1	A	242	LEU
1	A	246	ARG
1	A	260	ARG
1	A	280	PHE
1	A	285	GLN
1	A	292	TYR
1	A	298	LEU
1	A	304	LYS
1	A	314	GLU
1	A	318	GLN
1	A	332	LEU
1	A	339	GLN
1	A	347	MET
1	A	358	VAL
1	A	362	ILE
1	A	372	SER
1	A	379	VAL
1	A	389	GLN
1	A	408	MET
1	A	410	PHE
1	A	433	THR
1	A	466	ASP
1	A	467	ARG
1	A	475	ILE
1	A	479	PHE
1	A	498	ILE
1	A	529	LYS
1	A	544	ARG
1	A	546	GLN
1	A	548	THR
1	A	556	GLN
1	A	559	ARG

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Mol	Chain	Res	Type
1	A	561	LEU
1	A	587	THR
1	A	602	ASN
1	A	606	ASN
1	A	618	LEU
1	A	658	ARG
1	A	703	THR
1	A	731	GLU
1	A	735	SER
1	A	743	LYS
1	A	745	LEU
1	A	754	GLN
1	A	773	GLN
1	A	776	TYR
1	A	777	ILE
1	A	806	ARG
1	A	813	ARG
1	A	824	VAL
1	A	846	ILE
1	A	855	THR
1	A	861	ASP
1	A	880	LEU
1	A	893	LYS
1	B	9	GLU
1	B	22	SER
1	B	27	ARG
1	B	47	THR
1	B	61	LEU
1	B	83	LEU
1	B	86	ASP
1	B	90	LEU
1	B	93	LEU
1	B	115	ILE
1	B	116	GLU
1	B	130	LYS
1	B	145	ARG
1	B	146	PHE
1	B	147	TYR
1	B	164	ILE
1	B	177	GLU
1	B	181	GLU
1	B	218	VAL

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Mol	Chain	Res	Type
1	B	248	THR
1	B	249	ARG
1	B	257	TYR
1	B	260	ARG
1	B	274	ILE
1	B	280	PHE
1	B	291	ASP
1	B	378	LYS
1	B	382	GLN
1	B	386	HIS
1	B	388	VAL
1	B	392	PRO
1	B	421	ARG
1	B	436	VAL
1	B	451	SER
1	B	468	ASP
1	B	475	ILE
1	B	479	PHE
1	B	483	LYS
1	B	489	MET
1	B	499	ILE
1	B	525	GLU
1	B	570	LEU
1	B	632	ILE
1	B	658	ARG
1	B	668	ARG
1	B	685	ARG
1	B	686	GLU
1	B	703	THR
1	B	728	MET
1	B	734	LYS
1	B	742	GLN
1	B	758	GLU
1	B	766	GLU
1	B	773	GLN
1	B	809	LEU
1	B	843	ASP
1	B	856	ASP
1	B	894	LYS
1	C	7	THR
1	C	25	ARG
1	C	58	THR

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Mol	Chain	Res	Type
1	C	61	LEU
1	C	66	ARG
1	C	73	LYS
1	C	83	LEU
1	C	93	LEU
1	C	173	GLN
1	C	195	LYS
1	C	196	GLU
1	C	200	GLU
1	C	214	THR
1	C	218	VAL
1	C	247	LYS
1	C	255	ASN
1	C	256	MET
1	C	257	TYR
1	C	261	GLU
1	C	276	LEU
1	C	299	ASN
1	C	361	PRO
1	C	388	VAL
1	C	399	PRO
1	C	439	LEU
1	C	446	VAL
1	C	473	THR
1	C	474	GLU
1	C	483	LYS
1	C	490	LEU
1	C	525	GLU
1	C	556	GLN
1	C	559	ARG
1	C	561	LEU
1	C	562	LEU
1	C	587	THR
1	C	599	ARG
1	C	618	LEU
1	C	636	VAL
1	C	642	ARG
1	C	667	PHE
1	C	734	LYS
1	C	760	LEU
1	C	765	LYS
1	C	770	GLU

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Mol	Chain	Res	Type
1	C	819	ILE
1	C	820	ASP
1	C	830	VAL
1	C	843	ASP
1	C	856	ASP
1	C	880	LEU
1	C	898	PHE
1	D	2	LYS
1	D	10	GLN
1	D	32	GLU
1	D	41	CYS
1	D	47	THR
1	D	57	CYS
1	D	86	ASP
1	D	105	HIS
1	D	128	GLN
1	D	136	ILE
1	D	152	LEU
1	D	155	PRO
1	D	156	TYR
1	D	164	ILE
1	D	182	ILE
1	D	197	LEU
1	D	198	LEU
1	D	200	GLU
1	D	202	LEU
1	D	208	LYS
1	D	213	LEU
1	D	216	TRP
1	D	285	GLN
1	D	302	LYS
1	D	305	TYR
1	D	310	SER
1	D	362	ILE
1	D	363	LYS
1	D	407	VAL
1	D	452	ASP
1	D	456	CYS
1	D	474	GLU
1	D	479	PHE
1	D	484	GLU
1	D	485	HIS

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Mol	Chain	Res	Type
1	D	511	ASP
1	D	518	TYR
1	D	520	PHE
1	D	524	ASP
1	D	540	GLU
1	D	544	ARG
1	D	558	ASN
1	D	576	ARG
1	D	584	THR
1	D	591	GLN
1	D	592	MET
1	D	618	LEU
1	D	658	ARG
1	D	660	GLU
1	D	674	MET
1	D	702	TRP
1	D	703	THR
1	D	725	LEU
1	D	731	GLU
1	D	779	ILE
1	D	815	ILE
1	D	839	ASN
1	D	844	LYS
1	D	852	THR
1	D	873	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	23	ASN
1	A	40	HIS
1	A	64	ASN
1	A	112	ASN
1	A	153	ASN
1	A	158	ASN
1	A	171	GLN
1	A	228	ASN
1	A	284	ASN
1	A	285	GLN
1	A	333	GLN
1	A	342	ASN

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	422	GLN
1	A	495	ASN
1	A	505	ASN
1	A	546	GLN
1	A	556	GLN
1	A	572	ASN
1	A	602	ASN
1	A	606	ASN
1	A	645	ASN
1	A	646	HIS
1	A	678	GLN
1	A	733	GLN
1	A	773	GLN
1	A	786	ASN
1	A	812	ASN
1	A	818	ASN
1	A	864	HIS
1	B	40	HIS
1	B	70	GLN
1	B	138	HIS
1	B	153	ASN
1	B	171	GLN
1	B	173	GLN
1	B	193	ASN
1	B	206	GLN
1	B	207	GLN
1	B	232	ASN
1	B	245	HIS
1	B	284	ASN
1	B	354	GLN
1	B	356	GLN
1	B	376	GLN
1	B	377	ASN
1	B	382	GLN
1	B	389	GLN
1	B	424	ASN
1	B	495	ASN
1	B	505	ASN
1	B	539	ASN
1	B	556	GLN
1	B	558	ASN

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Mol	Chain	Res	Type
1	B	591	GLN
1	B	595	GLN
1	B	645	ASN
1	B	646	HIS
1	B	733	GLN
1	B	742	GLN
1	B	754	GLN
1	B	775	ASN
1	B	812	ASN
1	B	818	ASN
1	C	40	HIS
1	C	45	GLN
1	C	128	GLN
1	C	158	ASN
1	C	171	GLN
1	C	193	ASN
1	C	203	ASN
1	C	217	ASN
1	C	245	HIS
1	C	255	ASN
1	C	284	ASN
1	C	285	GLN
1	C	318	GLN
1	C	389	GLN
1	C	440	HIS
1	C	539	ASN
1	C	546	GLN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	595	GLN
1	C	646	HIS
1	C	675	ASN
1	C	678	GLN
1	C	711	ASN
1	C	761	GLN
1	C	787	ASN
1	C	818	ASN
1	D	70	GLN
1	D	128	GLN
1	D	171	GLN
1	D	173	GLN

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Mol	Chain	Res	Type
1	D	207	GLN
1	D	245	HIS
1	D	285	GLN
1	D	316	ASN
1	D	317	HIS
1	D	318	GLN
1	D	324	ASN
1	D	354	GLN
1	D	371	ASN
1	D	382	GLN
1	D	480	ASN
1	D	495	ASN
1	D	505	ASN
1	D	507	ASN
1	D	539	ASN
1	D	546	GLN
1	D	676	ASN
1	D	678	GLN
1	D	733	GLN
1	D	742	GLN
1	D	754	GLN
1	D	773	GLN
1	D	812	ASN
1	D	864	HIS

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	G	4	2,3	18,23,24	0.92	2 (11%)	21,35,38	1.14	2 (9%)
2	CTG	I	4	2,3	18,23,24	1.05	1 (5%)	21,35,38	1.29	3 (14%)
2	CTG	E	4	2,3	18,23,24	0.81	1 (5%)	21,35,38	1.09	2 (9%)

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	G	4	2,3	-	0/7/45/46	0/2/2/2
2	CTG	I	4	2,3	-	0/7/45/46	0/2/2/2
2	CTG	E	4	2,3	-	1/7/45/46	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C1'-N1	2.75	1.49	1.45
2	E	4	CTG	C1'-N1	2.41	1.48	1.45
2	G	4	CTG	C1'-N1	2.27	1.48	1.45
2	G	4	CTG	C5-C4	2.08	1.54	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	CTG	C2'-C1'-N1	-3.59	110.74	115.59
2	E	4	CTG	C2'-C1'-N1	-3.30	111.13	115.59
2	G	4	CTG	C2'-C1'-N1	-3.22	111.23	115.59
2	G	4	CTG	N3-C2-N1	-2.56	114.11	116.78
2	I	4	CTG	N3-C2-N1	-2.22	114.46	116.78
2	I	4	CTG	C2'-C3'-C4'	2.07	107.00	102.80
2	E	4	CTG	N3-C2-N1	-2.04	114.65	116.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	CTG	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	4	CTG	4	0
2	I	4	CTG	4	0
2	E	4	CTG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.21	13 (1%) 73 51	29, 63, 155, 176	0
1	B	902/906 (99%)	0.05	19 (2%) 63 40	30, 84, 172, 189	2 (0%)
1	C	901/906 (99%)	-0.27	4 (0%) 88 76	23, 64, 127, 148	0
1	D	890/906 (98%)	0.42	38 (4%) 40 21	57, 131, 173, 188	3 (0%)
2	E	17/18 (94%)	0.47	0 100 100	75, 106, 144, 148	0
2	G	17/18 (94%)	0.26	0 100 100	76, 113, 137, 147	0
2	I	17/18 (94%)	-0.27	0 100 100	39, 53, 124, 140	0
2	K	14/18 (77%)	0.63	2 (14%) 6 3	69, 156, 169, 170	0
3	F	14/14 (100%)	0.55	1 (7%) 22 11	85, 125, 157, 161	0
3	H	14/14 (100%)	0.44	0 100 100	89, 132, 155, 156	0
3	J	14/14 (100%)	-0.33	0 100 100	35, 55, 123, 127	0
3	L	13/14 (92%)	0.72	1 (7%) 19 10	146, 165, 169, 175	0
All	All	3715/3752 (99%)	0.01	78 (2%) 63 40	23, 83, 165, 189	5 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	862	VAL	9.1
1	D	847	ALA	4.4
1	D	858	ILE	4.1
1	B	503	LEU	4.0
1	A	858	ILE	3.9
1	D	799	PRO	3.9
1	A	847	ALA	3.9
1	D	776	TYR	3.8
1	D	863	LEU	3.8
1	D	846	ILE	3.6
1	A	863	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	851	GLY	3.5
1	A	855	THR	3.4
1	D	802	PRO	3.4
1	B	863	LEU	3.1
1	D	857	LEU	3.0
1	B	113	PHE	3.0
1	D	771	PHE	2.9
1	D	498	ILE	2.9
1	D	113	PHE	2.8
1	A	846	ILE	2.8
1	B	340	PHE	2.7
1	D	793	VAL	2.7
1	A	866	MET	2.7
1	B	846	ILE	2.6
1	D	800	LYS	2.6
1	B	170	LEU	2.6
1	B	277	TYR	2.6
3	F	101	DG	2.6
1	D	522	PHE	2.5
1	B	504	HIS	2.4
1	D	389	GLN	2.4
1	B	133	ILE	2.4
1	D	779	ILE	2.4
1	B	531	LYS	2.3
1	A	808	ILE	2.3
1	B	155	PRO	2.3
1	D	213	LEU	2.3
1	B	166	ILE	2.3
1	D	834	PRO	2.3
1	D	855	THR	2.3
1	C	514	LEU	2.2
1	D	850	SER	2.2
1	B	798	GLY	2.2
1	A	841	PHE	2.2
1	A	862	VAL	2.2
1	A	508	LEU	2.2
1	D	822	PRO	2.2
1	D	69	SER	2.2
1	B	324	ASN	2.2
2	K	5	DG	2.2
1	A	793	VAL	2.1
1	D	791	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	498	ILE	2.1
3	L	113	DC	2.1
2	K	6	DA	2.1
1	D	136	ILE	2.1
1	D	833	LEU	2.1
1	B	803	PHE	2.1
1	D	192	ASP	2.1
1	D	777	ILE	2.1
1	D	819	ILE	2.1
1	B	323	TYR	2.1
1	B	179	PRO	2.1
1	D	198	LEU	2.1
1	D	82	ALA	2.1
1	D	535	ALA	2.1
1	A	834	PRO	2.1
1	D	778	SER	2.1
1	D	531	LYS	2.1
1	D	508	LEU	2.1
1	D	514	LEU	2.0
1	B	864	HIS	2.0
1	C	244	PRO	2.0
1	C	513	PRO	2.0
1	B	197	LEU	2.0
1	C	303	LEU	2.0
1	D	115	ILE	2.0

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

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	G	4	22/23	0.77	0.12	122,128,129,129	0
2	CTG	E	4	22/23	0.82	0.12	109,113,124,125	0
2	CTG	I	4	22/23	0.94	0.09	72,78,81,81	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.