



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:25 AM UTC

PDB ID : 3RMA / pdb_00003rma
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing
Thymine Glycol
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.
Deposited on : 2011-04-20
Resolution : 2.84 Å(reported)

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

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

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

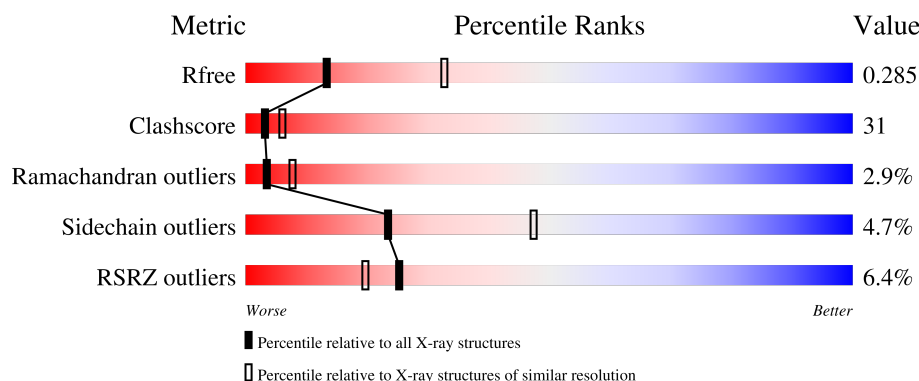
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	11% 56% 38% ..
1	B	906	11% 49% 44% 6% .
1	C	906	11% 56% 37% 6% .
1	D	906	12% 37% 53% 8% .
2	E	18	6% 22% 56% 22%

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Mol	Chain	Length	Quality of chain
2	G	18	6%6%61%6%28%
2	I	18	33%50%11%6%
2	K	18	17%50%33%
3	F	14	7%21%79%
3	H	14	14%21%71%7%
3	J	14	7%14%86%
3	L	14	21%71%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase.

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 4 is water.

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

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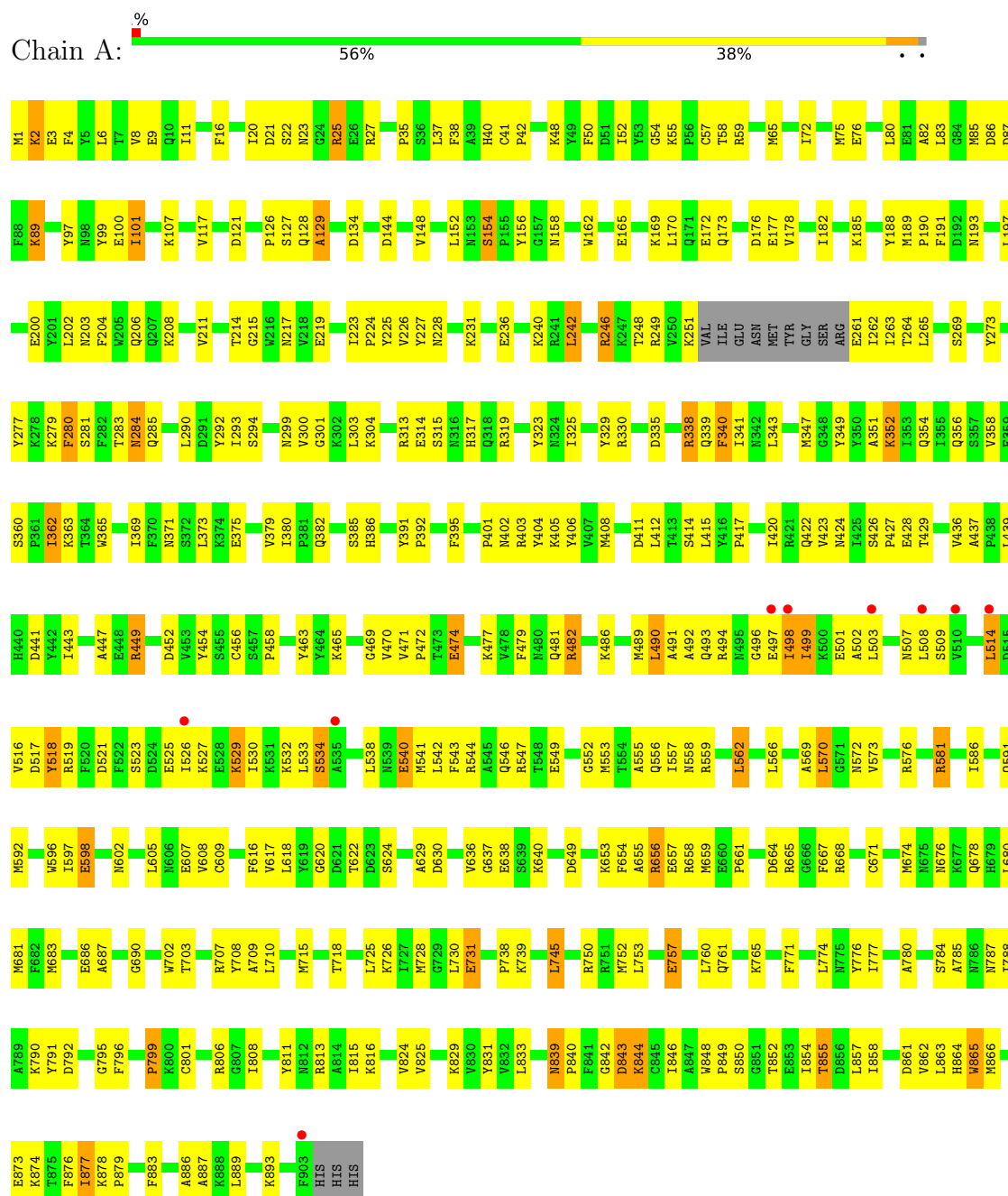
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	7	Total	O	0	0
			7	7		
4	J	6	Total	O	0	0
			6	6		
4	K	6	Total	O	0	0
			6	6		

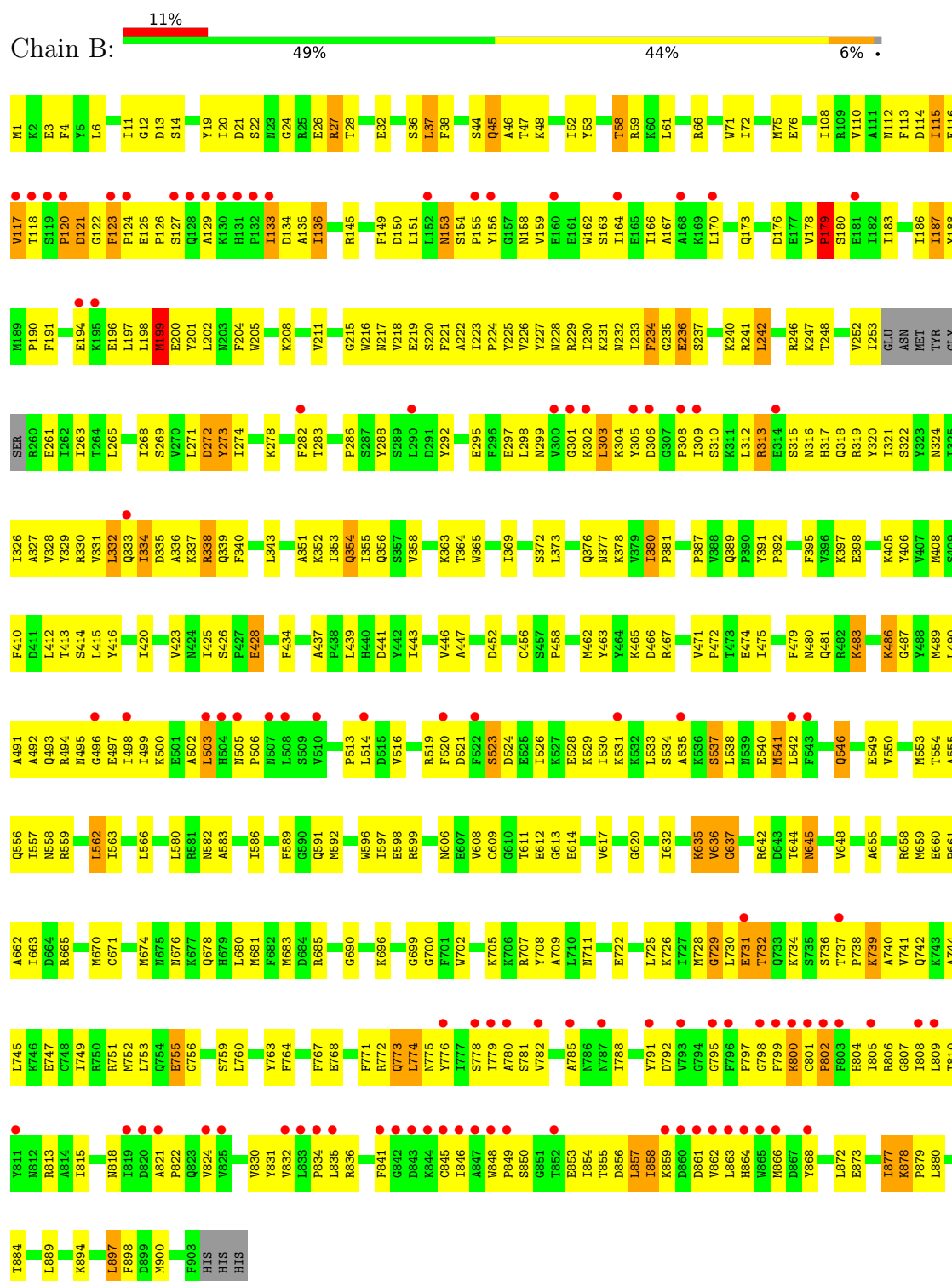
3 Residue-property plots

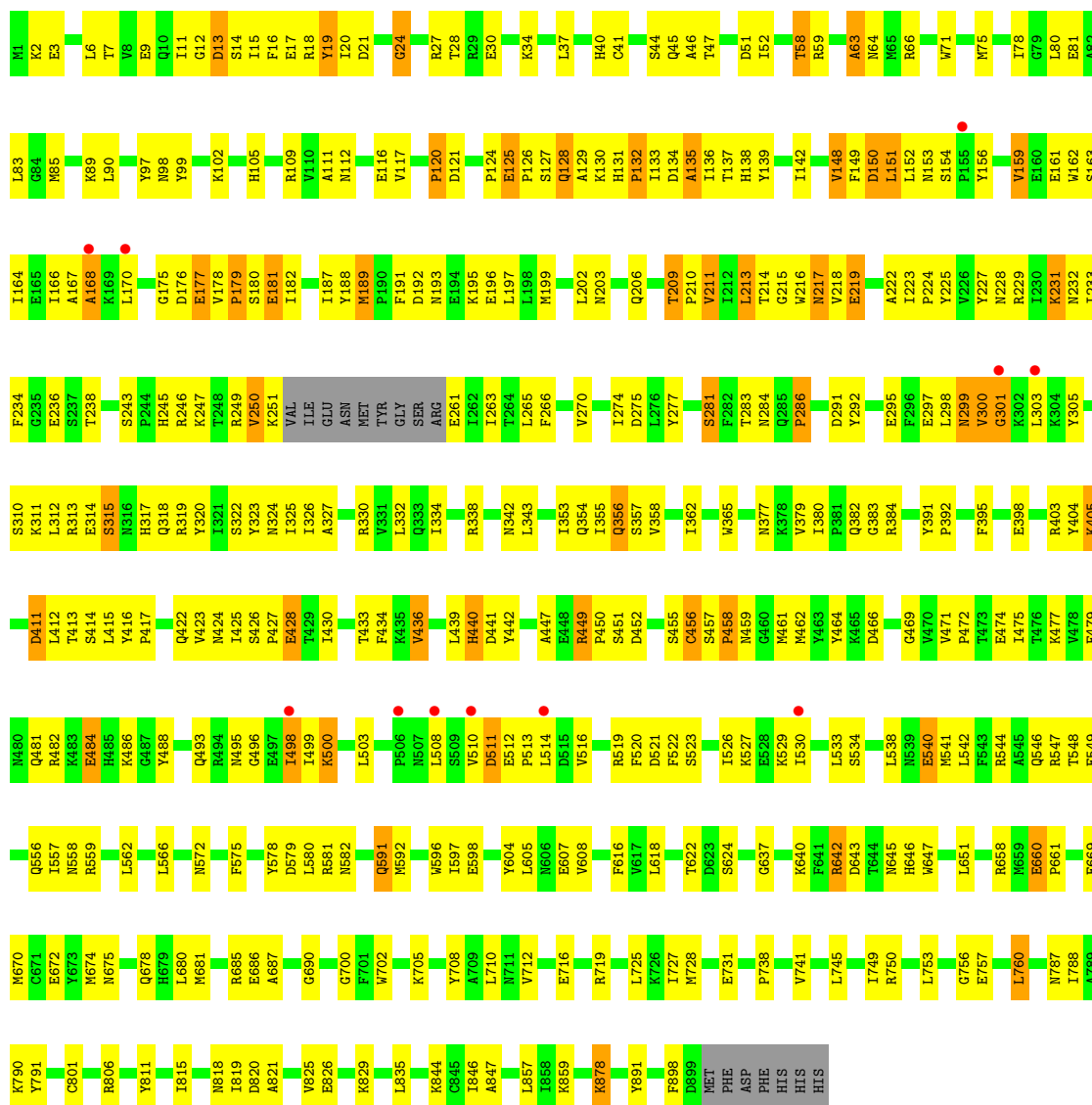
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

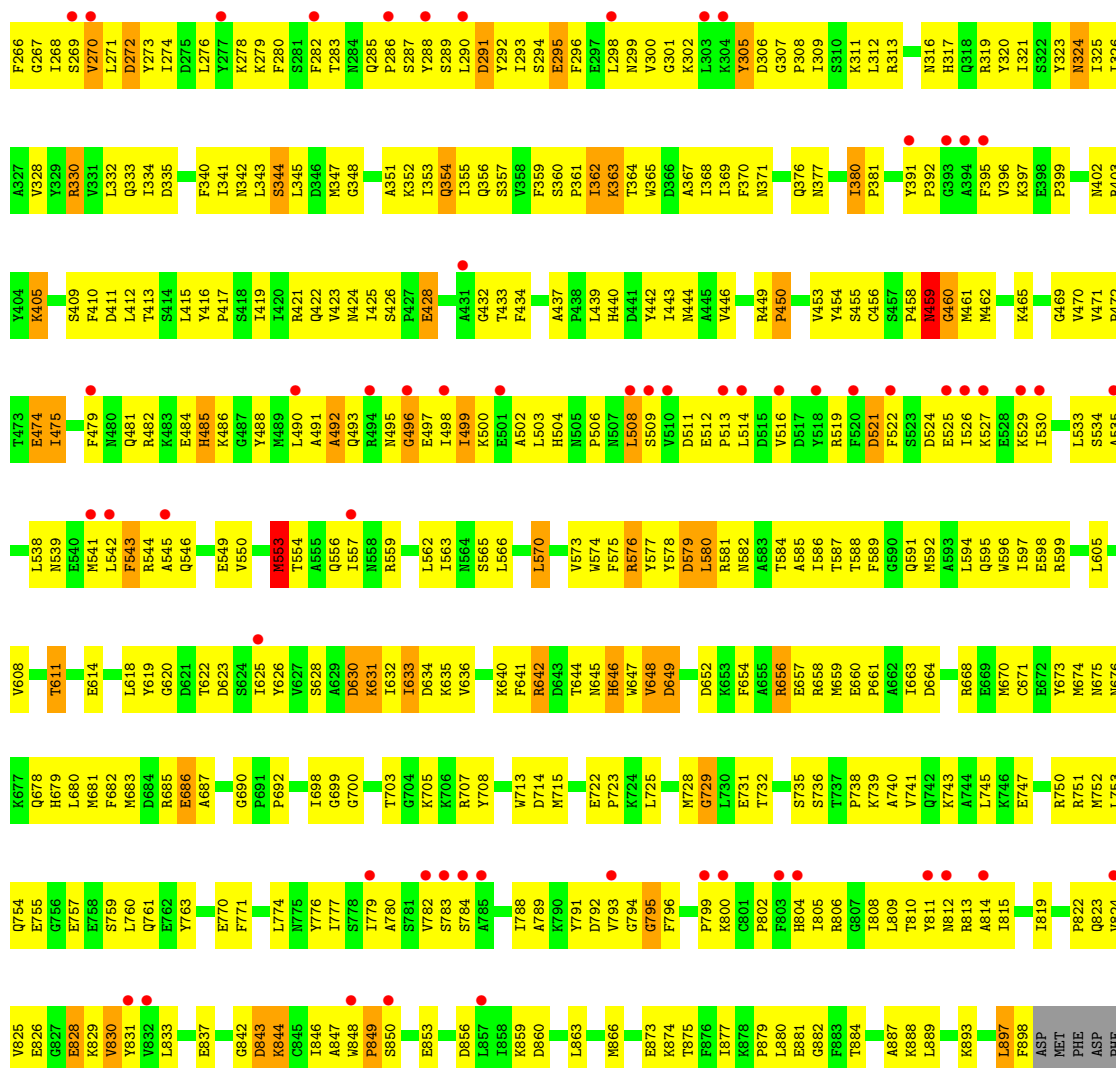
• Molecule 1: DNA polymerase



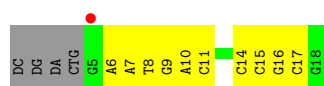
● Molecule 1: DNA polymerase



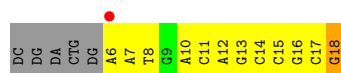
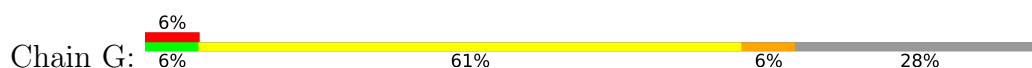




• Molecule 2: DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



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



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

Chain I:  33% 50% 11% 6%



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

Chain K:  17% 50% 33%



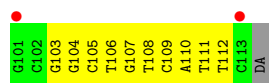
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain F:  7% 21% 79%



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

Chain H:  14% 21% 71% 7%



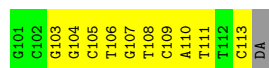
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain J:  7% 14% 86%



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

Chain L:  21% 71% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.70Å 123.00Å 163.94Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.84 50.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.84) 94.6 (50.00-2.84)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.275 0.229 , 0.285	Depositor DCC
R_{free} test set	23396 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31451	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.54	0/7452	1.02	32/10078 (0.3%)
1	B	0.46	0/7405	0.95	26/10021 (0.3%)
1	C	0.52	0/7404	0.98	32/10015 (0.3%)
1	D	0.37	0/7337	0.92	27/9939 (0.3%)
2	E	0.32	0/323	0.57	0/497
2	G	0.31	0/298	0.61	1/458 (0.2%)
2	I	0.41	0/371	0.78	1/569 (0.2%)
2	K	0.30	0/274	0.50	0/421
3	F	0.30	0/315	0.60	0/484
3	H	0.29	0/292	0.59	0/449
3	J	0.38	0/315	0.74	0/484
3	L	0.29	0/292	0.62	0/449
All	All	0.47	0/32078	0.95	119/43864 (0.3%)

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

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

There are no bond length outliers.

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-14.30	99.26	111.56
1	B	211	VAL	N-CA-C	-9.68	104.06	111.90
1	D	22	SER	N-CA-C	-9.26	101.08	111.82
1	C	436	VAL	N-CA-C	8.39	120.35	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	ASN	CA-C-N	8.12	127.78	119.82
1	A	839	ASN	C-N-CA	8.12	127.78	119.82
1	B	732	THR	N-CA-C	-7.82	102.38	112.23
1	A	178	VAL	N-CA-C	-7.76	101.95	108.63
1	B	632	ILE	N-CA-C	-7.53	103.52	110.82
1	D	830	VAL	N-CA-C	7.38	116.70	107.70
1	D	810	THR	N-CA-C	-7.33	104.32	113.55
1	C	825	VAL	N-CA-C	7.28	118.50	108.89
1	A	656	ARG	N-CA-C	7.19	119.11	111.28
1	D	648	VAL	N-CA-C	-7.14	103.72	113.00
1	C	211	VAL	N-CA-C	-7.13	104.81	111.45
1	B	648	VAL	N-CA-C	-7.13	103.58	110.42
1	D	324	ASN	N-CA-C	-7.10	103.88	112.54
1	C	859	LYS	N-CA-C	7.06	119.58	111.11
1	A	456	CYS	N-CA-C	7.00	120.53	109.81
1	C	405	LYS	N-CA-C	6.96	118.55	110.97
1	C	209	THR	CA-C-N	6.95	126.71	119.76
1	C	209	THR	C-N-CA	6.95	126.71	119.76
1	A	490	LEU	N-CA-C	-6.90	103.86	112.90
1	D	657	GLU	N-CA-C	6.80	121.03	112.87
1	D	504	HIS	N-CA-C	-6.79	103.94	111.82
1	D	492	ALA	N-CA-C	-6.60	105.79	114.31
1	D	499	ILE	N-CA-C	-6.60	104.73	112.98
1	D	635	LYS	N-CA-C	-6.54	104.19	111.71
1	D	814	ALA	N-CA-C	-6.52	105.62	113.97
1	C	125	GLU	CA-C-N	6.51	126.44	119.28
1	C	125	GLU	C-N-CA	6.51	126.44	119.28
1	D	496	GLY	N-CA-C	-6.48	106.83	115.32
1	D	432	GLY	N-CA-C	6.47	118.74	110.20
1	C	499	ILE	N-CA-C	-6.45	104.23	113.07
1	A	540	GLU	N-CA-C	-6.33	105.87	113.97
1	B	877	ILE	N-CA-C	6.28	116.44	110.53
1	D	502	ALA	N-CA-C	-6.24	105.31	113.17
1	D	101	ILE	N-CA-C	6.20	116.31	106.88
1	D	553	MET	N-CA-C	-6.19	104.70	112.93
1	A	340	PHE	N-CA-C	6.14	118.77	111.71
1	C	189	MET	CA-C-N	6.13	125.89	119.76
1	C	189	MET	C-N-CA	6.13	125.89	119.76
1	B	380	ILE	CA-C-N	6.12	126.08	120.21
1	B	380	ILE	C-N-CA	6.12	126.08	120.21
1	D	203	ASN	N-CA-C	-6.11	104.70	111.36
1	C	498	ILE	N-CA-C	-6.09	107.56	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	857	LEU	N-CA-C	-6.08	105.63	113.16
1	C	168	ALA	N-CA-C	-6.00	105.92	113.72
1	A	874	LYS	N-CA-C	5.99	117.89	111.36
1	A	55	LYS	CA-C-N	5.97	125.73	119.76
1	A	55	LYS	C-N-CA	5.97	125.73	119.76
1	B	354	GLN	N-CA-C	-5.96	101.59	110.23
1	B	465	LYS	N-CA-C	-5.96	106.17	113.50
1	C	263	ILE	N-CA-C	5.95	115.90	106.32
1	C	757	GLU	N-CA-C	5.94	118.24	111.11
1	A	486	LYS	N-CA-C	-5.92	104.90	111.71
1	A	129	ALA	N-CA-C	-5.91	103.24	111.39
1	A	236	GLU	N-CA-C	-5.90	104.98	111.82
1	B	503	LEU	N-CA-C	-5.89	106.09	113.28
1	C	540	GLU	N-CA-C	-5.88	106.44	113.97
1	C	449	ARG	CA-C-N	5.87	127.17	119.84
1	C	449	ARG	C-N-CA	5.87	127.17	119.84
1	D	703	THR	N-CA-C	-5.84	106.28	113.41
2	I	18	DG	C2'-C3'-O3'	-5.81	102.78	111.50
1	C	712	VAL	N-CA-C	5.79	116.91	108.58
1	B	153	ASN	N-CA-C	5.77	118.06	108.13
1	C	127	SER	N-CA-C	-5.75	106.25	113.20
1	C	806	ARG	N-CA-C	-5.75	105.02	111.28
1	A	449	ARG	CA-C-N	5.74	127.02	119.84
1	A	449	ARG	C-N-CA	5.74	127.02	119.84
1	B	531	LYS	N-CA-C	-5.71	106.07	113.16
1	C	305	TYR	N-CA-C	5.70	115.77	108.24
1	D	354	GLN	N-CA-C	-5.64	102.56	110.35
1	A	338	ARG	N-CA-C	5.62	119.23	112.38
1	A	703	THR	N-CA-C	-5.61	106.61	113.50
1	C	442	TYR	N-CA-C	-5.57	105.21	112.23
1	C	13	ASP	N-CA-C	-5.57	107.07	112.97
1	A	598	GLU	N-CA-C	-5.56	105.30	111.36
1	B	452	ASP	N-CA-C	-5.56	105.81	112.59
1	A	482	ARG	N-CA-C	-5.55	104.92	110.97
2	G	18	DG	C2'-C3'-O3'	-5.54	103.19	111.50
1	A	339	GLN	N-CA-C	5.53	119.20	111.90
1	B	798	GLY	CA-C-N	5.51	125.71	120.31
1	B	798	GLY	C-N-CA	5.51	125.71	120.31
1	D	794	GLY	N-CA-C	-5.46	108.48	115.42
1	D	543	PHE	N-CA-C	-5.46	105.72	112.38
1	B	313	ARG	N-CA-C	-5.45	104.99	111.69
1	C	756	GLY	N-CA-C	5.38	117.53	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	VAL	N-CA-C	-5.37	108.05	113.47
1	B	583	ALA	N-CA-C	-5.34	105.54	111.36
1	A	158	ASN	N-CA-C	-5.32	100.51	109.07
1	A	465	LYS	N-CA-C	-5.31	107.17	113.97
1	A	529	LYS	N-CA-C	-5.31	105.90	112.38
1	A	280	PHE	N-CA-C	5.30	119.92	112.72
1	A	865	TRP	N-CA-C	5.30	119.61	113.20
1	C	500	LYS	N-CA-C	-5.29	106.67	113.23
1	D	380	ILE	CA-C-N	5.28	126.44	119.84
1	D	380	ILE	C-N-CA	5.28	126.44	119.84
1	D	371	ASN	N-CA-C	5.25	116.69	111.07
1	B	437	ALA	N-CA-C	-5.24	104.11	110.13
1	B	242	LEU	N-CA-C	-5.20	106.91	113.20
1	C	403	ARG	N-CA-C	-5.19	102.07	110.32
1	A	877	ILE	N-CA-C	5.18	115.90	110.62
1	C	598	GLU	N-CA-C	-5.18	105.55	111.14
1	A	757	GLU	N-CA-C	5.17	117.31	111.11
1	B	546	GLN	N-CA-C	-5.15	107.16	113.50
1	B	806	ARG	N-CA-C	-5.15	106.26	112.54
1	B	332	LEU	N-CA-C	-5.13	105.81	111.71
1	B	446	VAL	N-CA-C	5.12	117.50	111.09
1	D	148	VAL	N-CA-C	5.11	116.17	109.58
1	C	150	ASP	N-CA-C	5.11	117.07	109.25
1	C	687	ALA	N-CA-C	5.11	118.06	110.14
1	D	19	TYR	N-CA-C	5.11	116.57	108.96
1	A	543	PHE	N-CA-C	-5.10	105.81	112.23
1	B	486	LYS	N-CA-C	-5.10	105.91	111.82
1	C	286	PRO	N-CA-C	-5.08	106.92	113.57
1	B	241	ARG	N-CA-C	-5.07	107.15	113.19
1	A	65	MET	N-CA-C	5.05	118.55	112.38
1	A	844	LYS	N-CA-C	5.04	116.62	111.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	7	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7273	0	7125	312	0
1	B	7230	0	7057	454	0
1	C	7227	0	7083	349	0
1	D	7161	0	6961	640	0
2	E	287	0	157	17	0
2	G	265	0	146	22	0
2	I	352	0	193	11	0
2	K	244	0	135	16	0
3	F	282	0	158	19	0
3	H	262	0	149	22	0
3	J	282	0	158	20	0
3	L	262	0	149	17	0
4	A	114	0	0	6	0
4	B	61	0	0	3	0
4	C	99	0	0	4	0
4	D	16	0	0	3	0
4	E	5	0	0	2	0
4	F	2	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	1	0
4	I	7	0	0	1	0
4	J	6	0	0	0	0
4	K	6	0	0	1	0
All	All	31451	0	29471	1872	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 31.

All (1872) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:H	1:A:2:LYS:HD2	1.13	1.10
1:D:422:GLN:HE22	1:D:681:MET:HG2	1.15	1.09
1:D:481:GLN:HB3	1:D:559:ARG:HE	1.14	1.07
2:K:16:DG:H2''	2:K:17:DC:H5''	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:ASN:HD21	1:B:857:LEU:HD11	1.17	1.05
1:B:731:GLU:HA	1:B:734:LYS:HG2	1.39	1.04
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.32	1.04
1:B:707:ARG:HE	2:G:8:DT:H4'	1.18	1.04
1:D:543:PHE:HA	1:D:546:GLN:HE21	1.20	1.02
1:A:85:MET:HE2	1:A:87:ASP:H	1.24	1.01
1:D:90:LEU:HD11	1:D:353:ILE:HG22	1.43	1.01
1:D:516:VAL:HG11	1:D:526:ILE:HG21	1.42	1.00
1:B:136:ILE:HG23	1:B:149:PHE:HB2	1.42	0.98
1:D:295:GLU:HG2	1:D:301:GLY:HA2	1.43	0.97
1:A:857:LEU:HD12	1:A:858:ILE:HG23	1.46	0.96
1:A:395:PHE:HB2	1:A:591:GLN:HG3	1.47	0.96
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.43	0.96
1:C:482:ARG:HE	1:C:556:GLN:HE21	1.13	0.96
1:A:482:ARG:NE	1:A:556:GLN:HE21	1.64	0.96
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.47	0.96
1:C:130:LYS:HG3	1:C:131:HIS:H	1.28	0.95
1:D:859:LYS:HG3	1:D:860:ASP:H	1.30	0.95
1:B:481:GLN:HE21	1:B:559:ARG:HE	1.08	0.95
1:D:112:ASN:HB3	1:D:214:THR:HG23	1.45	0.95
1:D:500:LYS:HA	1:D:503:LEU:HB2	1.49	0.95
1:B:395:PHE:HB2	1:B:591:GLN:HG2	1.49	0.94
1:C:395:PHE:HB2	1:C:591:GLN:HG3	1.49	0.94
1:B:606:ASN:HD21	1:B:614:GLU:H	1.15	0.94
1:A:482:ARG:HE	1:A:556:GLN:HE21	0.98	0.94
1:B:815:ILE:HD11	1:B:855:THR:HG21	1.50	0.94
1:C:354:GLN:HB3	1:C:356:GLN:HE22	1.33	0.94
1:B:387:PRO:HG2	1:B:389:GLN:HE21	1.30	0.93
1:C:461:MET:HE3	1:C:581:ARG:HB3	1.47	0.93
3:L:108:DT:H2''	3:L:109:DC:H5''	1.51	0.93
2:K:15:DC:H2''	2:K:16:DG:C8	2.04	0.92
1:D:573:VAL:HG23	1:D:574:TRP:HD1	1.35	0.92
2:G:10:DA:H2''	2:G:11:DC:H5'	1.51	0.92
2:K:10:DA:H2''	2:K:11:DC:H5''	1.53	0.91
1:A:514:LEU:HD12	1:A:530:ILE:HG12	1.53	0.91
1:C:249:ARG:HD3	1:C:251:LYS:HZ3	1.35	0.91
1:D:449:ARG:HH21	1:D:675:ASN:HB2	1.36	0.91
1:C:486:LYS:HB2	1:C:556:GLN:HG3	1.53	0.91
2:E:10:DA:H2''	2:E:11:DC:H5'	1.54	0.90
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.53	0.89
1:D:482:ARG:HB2	1:D:559:ARG:HB3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLU:HB3	1:D:11:ILE:HD11	1.56	0.87
3:F:104:DG:H1'	3:F:105:DC:H5''	1.55	0.87
1:D:261:GLU:HG3	1:D:262:ILE:HG13	1.54	0.87
1:D:752:MET:HG2	1:D:760:LEU:HD12	1.58	0.86
1:D:481:GLN:CB	1:D:559:ARG:HE	1.89	0.86
1:D:543:PHE:HA	1:D:546:GLN:NE2	1.89	0.86
1:B:606:ASN:HD22	1:B:612:GLU:HA	1.39	0.86
1:D:118:THR:HB	1:D:313:ARG:HE	1.40	0.85
1:D:288:TYR:HA	1:D:293:ILE:HD11	1.57	0.85
1:B:170:LEU:HB2	1:B:173:GLN:HE21	1.42	0.85
1:D:206:GLN:HE22	1:D:241:ARG:HB3	1.42	0.85
1:B:894:LYS:HA	4:B:918:HOH:O	1.77	0.84
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.42	0.84
1:B:163:SER:H	1:B:318:GLN:HE22	1.22	0.84
1:D:812:ASN:HA	1:D:815:ILE:HG12	1.60	0.84
1:A:3:GLU:HG2	1:A:21:ASP:HA	1.60	0.84
1:C:645:ASN:HD21	1:C:719:ARG:HD2	1.42	0.84
1:A:449:ARG:HH12	1:A:452:ASP:HB3	1.42	0.83
1:B:897:LEU:HD23	1:B:897:LEU:H	1.41	0.83
1:B:707:ARG:NE	2:G:8:DT:H4'	1.93	0.83
1:D:81:GLU:OE1	1:D:83:LEU:HD21	1.77	0.83
1:B:115:ILE:HG12	1:B:116:GLU:H	1.44	0.82
1:D:656:ARG:HA	1:D:660:GLU:OE2	1.79	0.82
1:B:145:ARG:HD2	1:B:187:ILE:HD11	1.60	0.82
3:J:113:DC:H2''	3:J:114:DA:H5''	1.61	0.82
3:H:104:DG:H2''	3:H:105:DC:H5''	1.62	0.82
1:C:495:ASN:HD21	1:C:521:ASP:HA	1.44	0.81
1:B:217:ASN:HB2	1:B:274:ILE:HD12	1.62	0.81
1:B:502:ALA:HB3	1:B:530:ILE:HG12	1.61	0.81
1:D:222:ALA:O	1:D:226:VAL:HG23	1.80	0.81
1:D:503:LEU:O	1:D:506:PRO:HD3	1.81	0.81
1:A:499:ILE:HD13	1:A:541:MET:HG3	1.61	0.81
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.62	0.81
1:C:424:ASN:HD21	1:C:469:GLY:H	1.24	0.81
1:A:206:GLN:HE22	1:A:246:ARG:NH2	1.79	0.80
1:B:493:GLN:HB3	1:B:549:GLU:OE2	1.81	0.80
1:D:271:LEU:HB3	1:D:276:LEU:HD11	1.60	0.80
1:D:402:ASN:ND2	1:D:403:ARG:H	1.80	0.80
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.46	0.80
1:D:302:LYS:HE3	1:D:323:TYR:HE2	1.45	0.80
1:D:395:PHE:HB2	1:D:591:GLN:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ARG:HG2	1:C:547:ARG:HH21	1.47	0.79
1:D:831:TYR:HD2	1:D:848:TRP:HE1	1.27	0.79
1:D:361:PRO:HB3	1:D:565:SER:HB2	1.65	0.79
1:C:249:ARG:HD3	1:C:251:LYS:NZ	1.96	0.79
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.63	0.79
1:C:382:GLN:HG2	1:C:383:GLY:N	1.98	0.79
2:K:16:DG:C2'	2:K:17:DC:H5''	2.13	0.79
1:C:216:TRP:O	1:C:217:ASN:HB2	1.82	0.79
1:D:298:LEU:HB2	1:D:300:VAL:HG12	1.63	0.79
1:D:542:LEU:O	1:D:546:GLN:HG3	1.83	0.79
2:G:15:DC:H2'	2:G:16:DG:C8	2.17	0.79
1:B:115:ILE:HD11	1:B:133:ILE:HG12	1.65	0.79
1:D:434:PHE:CE1	1:D:460:GLY:HA2	2.18	0.79
3:L:108:DT:C2'	3:L:109:DC:H5''	2.13	0.78
1:C:382:GLN:HG2	1:C:383:GLY:H	1.46	0.78
1:D:236:GLU:HA	1:D:239:ALA:HB3	1.66	0.78
1:D:6:LEU:HG	1:D:19:TYR:HA	1.63	0.78
1:D:308:PRO:HG2	1:D:311:LYS:HB2	1.64	0.77
1:B:123:PHE:CE1	1:B:309:ILE:HD11	2.19	0.77
1:C:461:MET:HE1	1:C:581:ARG:HD2	1.66	0.77
1:A:428:GLU:OE2	1:A:470:VAL:HG23	1.85	0.77
1:C:219:GLU:HG3	1:C:270:VAL:HG11	1.66	0.77
1:D:516:VAL:HG21	1:D:522:PHE:CZ	2.20	0.77
1:A:249:ARG:HH11	1:A:251:LYS:HE2	1.49	0.77
1:B:115:ILE:HD11	1:B:133:ILE:CG1	2.15	0.77
1:D:825:VAL:HB	1:D:828:GLU:HB2	1.66	0.76
1:B:854:ILE:HD13	1:B:862:VAL:HG11	1.67	0.76
1:D:830:VAL:HG23	1:D:848:TRP:O	1.85	0.76
1:B:785:ALA:HB1	1:B:788:ILE:HD11	1.67	0.76
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.21	0.76
3:F:108:DT:H2''	3:F:109:DC:H5''	1.66	0.76
1:A:283:THR:O	1:A:285:GLN:HG2	1.85	0.76
1:D:205:TRP:NE1	1:D:242:LEU:HA	2.01	0.76
3:H:104:DG:H2''	3:H:105:DC:C5'	2.15	0.76
1:C:130:LYS:HG3	1:C:131:HIS:N	2.01	0.76
1:A:314:GLU:HG3	1:A:315:SER:N	2.00	0.76
1:D:461:MET:HE1	1:D:581:ARG:HH21	1.50	0.76
1:A:482:ARG:HE	1:A:556:GLN:NE2	1.81	0.76
1:B:776:TYR:HB3	1:B:863:LEU:HD13	1.68	0.76
1:D:644:THR:O	1:D:648:VAL:HG23	1.86	0.76
1:D:859:LYS:HG3	1:D:860:ASP:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:DA:H2''	2:G:11:DC:C5'	2.16	0.76
1:A:72:ILE:O	1:A:76:GLU:HG3	1.86	0.75
1:C:481:GLN:HE21	1:C:559:ARG:HE	1.32	0.75
1:D:530:ILE:HG13	1:D:533:LEU:HD22	1.68	0.75
1:B:533:LEU:HB2	1:B:538:LEU:HD13	1.67	0.75
1:A:602:ASN:HD21	1:A:617:VAL:H	1.35	0.75
1:B:163:SER:HB3	1:B:166:ILE:HB	1.68	0.75
1:B:736:SER:HA	1:B:782:VAL:HB	1.68	0.75
1:B:752:MET:HE3	1:B:889:LEU:HD12	1.69	0.75
1:D:295:GLU:CG	1:D:301:GLY:HA2	2.16	0.75
1:A:281:SER:HB2	1:A:338:ARG:HH21	1.52	0.74
1:A:290:LEU:O	1:A:294:SER:HB2	1.86	0.74
1:B:322:SER:O	1:B:326:ILE:HG12	1.87	0.74
1:C:303:LEU:HD23	1:C:323:TYR:HB2	1.69	0.74
1:D:229:ARG:HG3	1:D:233:ILE:HD11	1.69	0.74
1:A:502:ALA:O	1:A:538:LEU:HD13	1.87	0.74
1:B:115:ILE:HG12	1:B:116:GLU:N	2.01	0.74
1:C:326:ILE:HD12	1:C:327:ALA:N	2.03	0.74
2:E:6:DA:H1'	2:E:7:DA:H5''	1.70	0.74
1:A:526:ILE:HG22	1:A:530:ILE:HD11	1.69	0.74
1:B:897:LEU:HD12	1:D:636:VAL:HG11	1.68	0.74
1:D:15:ILE:HD12	1:D:92:TYR:CE2	2.21	0.74
1:D:145:ARG:HG3	1:D:185:LYS:O	1.88	0.74
2:K:10:DA:C2'	2:K:11:DC:H5''	2.17	0.74
1:D:411:ASP:HB2	1:D:686:GLU:OE1	1.88	0.74
1:B:481:GLN:HE21	1:B:559:ARG:NE	1.82	0.73
1:D:25:ARG:HH11	1:D:25:ARG:HG3	1.53	0.73
1:D:85:MET:HE2	1:D:87:ASP:HB3	1.70	0.73
1:B:658:ARG:HD2	1:D:897:LEU:HD22	1.70	0.73
1:C:78:ILE:HG13	1:C:80:LEU:HD23	1.70	0.73
1:D:343:LEU:HD23	1:D:554:THR:HG23	1.67	0.73
1:D:805:ILE:HA	1:D:808:ILE:HD12	1.71	0.73
1:B:170:LEU:HB2	1:B:173:GLN:NE2	2.04	0.73
1:D:109:ARG:HD2	1:D:209:THR:O	1.88	0.73
1:D:751:ARG:HD3	1:D:759:SER:OG	1.87	0.73
2:K:10:DA:H2''	2:K:11:DC:C5'	2.19	0.73
3:L:108:DT:H2''	3:L:109:DC:C5'	2.19	0.73
1:B:116:GLU:HG3	1:B:135:ALA:HB3	1.69	0.72
1:D:525:GLU:O	1:D:529:LYS:HE2	1.89	0.72
1:A:362:ILE:HD12	1:A:569:ALA:HA	1.71	0.72
1:A:428:GLU:N	1:A:428:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ARG:NH1	1:A:452:ASP:HB3	2.04	0.72
1:B:738:PRO:HG2	1:B:741:VAL:HB	1.71	0.72
1:D:654:PHE:O	1:D:658:ARG:HB2	1.88	0.72
3:H:104:DG:C2'	3:H:105:DC:H5''	2.19	0.72
1:B:486:LYS:HG3	1:B:556:GLN:OE1	1.88	0.72
1:D:271:LEU:HD22	1:D:276:LEU:HD21	1.69	0.72
1:B:327:ALA:O	1:B:331:VAL:HG23	1.90	0.72
1:D:151:LEU:HD23	1:D:152:LEU:N	2.05	0.72
1:B:731:GLU:HA	1:B:734:LYS:CG	2.18	0.72
1:D:66:ARG:O	1:D:70:GLN:HG2	1.89	0.72
1:A:842:GLY:O	1:A:843:ASP:HB2	1.90	0.72
1:D:508:LEU:HD22	1:D:508:LEU:H	1.55	0.72
1:D:461:MET:CE	1:D:581:ARG:HH21	2.02	0.72
1:A:530:ILE:O	1:A:533:LEU:HD13	1.90	0.71
1:C:163:SER:H	1:C:318:GLN:HE22	1.36	0.71
1:A:687:ALA:HB2	1:A:715:MET:HE1	1.72	0.71
1:C:354:GLN:HB3	1:C:356:GLN:NE2	2.05	0.71
3:J:104:DG:H1'	3:J:105:DC:H5''	1.71	0.71
1:D:481:GLN:HB3	1:D:559:ARG:NE	1.98	0.71
1:D:302:LYS:HE3	1:D:323:TYR:CE2	2.26	0.71
1:D:313:ARG:HD3	1:D:320:TYR:CE2	2.26	0.71
1:D:85:MET:HE2	1:D:87:ASP:H	1.53	0.71
1:A:362:ILE:CD1	1:A:569:ALA:HA	2.21	0.71
1:D:433:THR:HG22	1:D:461:MET:HE3	1.71	0.71
3:J:108:DT:H2''	3:J:109:DC:H5'	1.71	0.71
1:A:449:ARG:HH12	1:A:452:ASP:CB	2.04	0.71
1:B:330:ARG:O	1:B:334:ILE:HG22	1.90	0.71
1:A:347:MET:HE3	1:A:558:ASN:ND2	2.06	0.71
1:B:795:GLY:O	1:B:813:ARG:HD3	1.91	0.71
1:D:316:ASN:HD22	1:D:319:ARG:HB3	1.56	0.71
1:D:330:ARG:O	1:D:334:ILE:HG13	1.91	0.71
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.72	0.70
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.73	0.70
1:D:550:VAL:HA	1:D:553:MET:HB3	1.73	0.70
2:E:6:DA:H2''	2:E:7:DA:H5'	1.72	0.70
1:C:815:ILE:HD12	1:C:821:ALA:CB	2.21	0.70
1:D:229:ARG:O	1:D:233:ILE:HG13	1.90	0.70
1:D:360:SER:HB2	1:D:363:LYS:HB2	1.73	0.70
1:A:206:GLN:HE22	1:A:246:ARG:HH22	1.39	0.70
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.26	0.70
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:16:DG:H2''	2:G:17:DC:C5'	2.22	0.70
1:B:818:ASN:ND2	1:B:857:LEU:HD11	2.01	0.70
1:D:160:GLU:HG3	1:D:161:GLU:H	1.57	0.70
1:D:422:GLN:NE2	1:D:681:MET:HG2	2.00	0.70
1:A:172:GLU:H	1:A:172:GLU:CD	1.99	0.70
1:A:422:GLN:NE2	1:A:680:LEU:H	1.89	0.70
1:B:334:ILE:HG13	1:B:338:ARG:HG3	1.73	0.70
1:C:356:GLN:H	1:C:356:GLN:HE21	1.40	0.70
1:D:359:PHE:O	1:D:361:PRO:HD3	1.92	0.70
1:B:1:MET:HE1	1:B:24:GLY:HA2	1.74	0.69
1:B:513:PRO:HG2	1:B:540:GLU:HG3	1.74	0.69
1:D:137:THR:H	1:D:324:ASN:HD21	1.38	0.69
1:B:744:ALA:HB2	1:B:767:PHE:CE2	2.28	0.69
1:D:479:PHE:HA	1:D:563:ILE:HD11	1.74	0.69
2:E:10:DA:H2''	2:E:11:DC:C5'	2.22	0.69
1:D:191:PHE:CD2	1:D:197:LEU:HA	2.27	0.69
1:A:224:PRO:HA	1:A:263:ILE:HD13	1.75	0.69
1:B:136:ILE:CG2	1:B:149:PHE:HB2	2.19	0.69
1:B:554:THR:HA	1:B:557:ILE:HG22	1.75	0.69
1:C:645:ASN:ND2	1:C:719:ARG:HD2	2.08	0.69
1:D:198:LEU:HD23	1:D:230:ILE:HG12	1.75	0.69
1:D:305:TYR:CG	1:D:312:LEU:HD22	2.27	0.69
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.08	0.69
1:D:191:PHE:CZ	1:D:200:GLU:HB3	2.27	0.69
1:D:642:ARG:HD2	1:D:646:HIS:CE1	2.28	0.69
1:A:558:ASN:O	1:A:562:LEU:HD22	1.93	0.68
1:B:72:ILE:O	1:B:76:GLU:HG3	1.92	0.68
1:B:188:TYR:CZ	1:B:190:PRO:HB3	2.28	0.68
1:B:846:ILE:HG21	1:B:862:VAL:HG23	1.75	0.68
1:D:205:TRP:HE1	1:D:242:LEU:HA	1.59	0.68
1:D:402:ASN:HD22	1:D:403:ARG:H	1.42	0.68
1:B:272:ASP:OD1	1:B:274:ILE:HG22	1.94	0.68
1:B:481:GLN:NE2	1:B:559:ARG:HE	1.88	0.68
1:C:461:MET:HE2	4:C:958:HOH:O	1.92	0.68
1:D:402:ASN:ND2	1:D:403:ARG:HG2	2.08	0.68
1:A:281:SER:HB2	1:A:338:ARG:NH2	2.08	0.68
1:D:189:MET:HE1	1:D:200:GLU:HG2	1.75	0.68
1:D:738:PRO:HB3	1:D:780:ALA:O	1.92	0.68
1:B:554:THR:HA	1:B:557:ILE:CG2	2.24	0.68
1:A:261:GLU:O	1:A:262:ILE:HD12	1.95	0.67
1:A:281:SER:O	1:A:283:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB1	1:B:225:TYR:CE2	2.29	0.67
1:D:31:VAL:HG12	1:D:32:GLU:N	2.08	0.67
1:D:793:VAL:HG22	1:D:796:PHE:O	1.94	0.67
1:A:197:LEU:HD23	1:A:197:LEU:C	2.20	0.67
1:A:402:ASN:HA	1:A:886:ALA:O	1.93	0.67
3:F:108:DT:H2''	3:F:109:DC:C5'	2.24	0.67
1:C:83:LEU:HD12	1:C:83:LEU:N	2.09	0.67
1:D:403:ARG:HD2	1:D:887:ALA:O	1.93	0.67
1:B:116:GLU:CG	1:B:135:ALA:HB3	2.25	0.67
1:D:316:ASN:ND2	1:D:319:ARG:HB3	2.10	0.67
1:C:818:ASN:ND2	1:C:857:LEU:HD11	2.10	0.67
1:D:109:ARG:CZ	1:D:142:ILE:HD11	2.25	0.67
1:D:434:PHE:HE1	1:D:461:MET:H	1.41	0.67
1:C:152:LEU:HD11	1:C:161:GLU:HG2	1.76	0.66
1:D:340:PHE:HD1	1:D:343:LEU:HD12	1.60	0.66
1:A:855:THR:HG23	1:A:858:ILE:HG12	1.77	0.66
1:C:645:ASN:ND2	1:C:719:ARG:HH11	1.93	0.66
1:D:7:THR:HG22	1:D:18:ARG:HB2	1.78	0.66
1:D:219:GLU:OE2	1:D:262:ILE:HG23	1.94	0.66
1:D:453:VAL:HG23	1:D:454:TYR:CD2	2.30	0.66
2:G:15:DC:H42	3:H:103:DG:H1	1.43	0.66
1:A:2:LYS:HD2	1:A:2:LYS:N	1.97	0.66
1:A:82:ALA:O	1:A:382:GLN:HB2	1.95	0.66
1:A:474:GLU:OE2	1:A:477:LYS:HE2	1.95	0.66
1:D:1:MET:HE3	1:D:102:LYS:HE3	1.76	0.66
3:F:103:DG:H2''	3:F:104:DG:H5'	1.78	0.66
1:B:848:TRP:CE3	1:B:854:ILE:HD12	2.31	0.66
1:C:166:ILE:HG22	1:C:175:GLY:HA2	1.76	0.66
1:D:124:PRO:HB3	1:D:131:HIS:HD2	1.61	0.66
1:D:212:ILE:O	1:D:212:ILE:HG22	1.96	0.66
1:D:365:TRP:CE2	1:D:566:LEU:HD23	2.31	0.66
1:D:611:THR:HB	1:D:614:GLU:OE1	1.96	0.66
1:B:14:SER:HB3	1:B:32:GLU:OE2	1.95	0.66
1:D:399:PRO:HB3	1:D:619:TYR:CD2	2.31	0.66
1:B:229:ARG:NE	1:B:233:ILE:HD11	2.10	0.65
1:B:316:ASN:ND2	1:B:319:ARG:H	1.93	0.65
1:D:273:TYR:HA	1:D:276:LEU:HD12	1.76	0.65
1:D:831:TYR:HD2	1:D:848:TRP:NE1	1.94	0.65
1:D:458:PRO:HB2	1:D:588:THR:HG22	1.77	0.65
1:C:512:GLU:HB3	1:C:513:PRO:HD2	1.78	0.65
1:C:642:ARG:HD2	1:C:646:HIS:NE2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:16:DG:H2''	2:K:17:DC:C5'	2.21	0.65
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.26	0.65
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.79	0.65
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.77	0.65
1:B:331:VAL:O	1:B:334:ILE:HG23	1.97	0.65
1:D:31:VAL:HG12	1:D:32:GLU:H	1.59	0.65
1:D:305:TYR:OH	1:D:309:ILE:HB	1.95	0.65
2:G:13:DG:H1	3:H:105:DC:H42	1.43	0.65
2:G:15:DC:H4'	2:G:15:DC:OP1	1.97	0.65
1:A:653:LYS:HD3	1:A:656:ARG:HH22	1.61	0.65
1:C:534:SER:O	1:C:538:LEU:HG	1.97	0.65
1:B:52:ILE:HD12	1:B:428:GLU:HG3	1.79	0.65
1:B:316:ASN:HD21	1:B:318:GLN:HB3	1.62	0.65
1:C:660:GLU:CB	1:C:661:PRO:HD3	2.27	0.65
1:A:85:MET:HA	1:A:85:MET:HE3	1.79	0.65
1:A:280:PHE:CD1	1:A:343:LEU:HD23	2.31	0.65
1:B:495:ASN:OD1	1:B:521:ASP:HA	1.97	0.65
1:D:137:THR:H	1:D:324:ASN:ND2	1.95	0.65
1:D:197:LEU:O	1:D:197:LEU:HD23	1.96	0.65
1:D:530:ILE:HA	1:D:533:LEU:HD13	1.77	0.65
3:L:110:DA:H1'	3:L:111:DT:H5''	1.76	0.65
1:C:486:LYS:HD3	1:C:556:GLN:NE2	2.12	0.65
1:C:818:ASN:HD22	1:C:821:ALA:H	1.45	0.65
3:J:104:DG:H2''	3:J:105:DC:C5'	2.27	0.65
1:B:123:PHE:CG	1:B:124:PRO:HD2	2.32	0.64
1:D:348:GLY:HA3	1:D:355:ILE:HD13	1.79	0.64
2:G:16:DG:H2''	2:G:17:DC:H5''	1.79	0.64
1:D:283:THR:CG2	1:D:285:GLN:HE22	2.09	0.64
1:D:353:ILE:HG13	1:D:354:GLN:O	1.96	0.64
1:D:802:PRO:HG2	1:D:805:ILE:CG1	2.27	0.64
2:E:14:DC:H2''	2:E:15:DC:O5'	1.97	0.64
1:B:808:ILE:HD11	1:B:830:VAL:HG21	1.80	0.64
1:D:248:THR:HG23	1:D:264:THR:O	1.96	0.64
1:D:740:ALA:O	1:D:743:LYS:HG2	1.97	0.64
1:D:825:VAL:HG12	1:D:826:GLU:N	2.12	0.64
1:D:131:HIS:HB2	1:D:225:TYR:OH	1.97	0.64
1:B:412:LEU:HD13	1:B:415:LEU:HD13	1.80	0.64
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.79	0.64
1:D:85:MET:HE2	1:D:87:ASP:CB	2.27	0.64
1:D:594:LEU:O	1:D:598:GLU:HG3	1.98	0.64
1:A:489:MET:SD	1:A:553:MET:HG2	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:CZ	1:B:233:ILE:HD11	2.28	0.64
1:D:271:LEU:HD13	1:D:276:LEU:HD21	1.79	0.64
1:A:314:GLU:CG	1:A:315:SER:N	2.61	0.64
1:B:164:ILE:HG22	1:B:183:ILE:HD11	1.79	0.64
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.80	0.64
1:D:148:VAL:HG21	1:D:325:ILE:HD11	1.80	0.64
1:A:269:SER:OG	1:A:356:GLN:NE2	2.31	0.64
1:B:167:ALA:HB1	1:B:178:VAL:HG23	1.80	0.64
1:C:411:ASP:OD1	1:C:624:SER:HB3	1.98	0.64
1:D:191:PHE:HZ	1:D:200:GLU:HB3	1.61	0.64
1:D:812:ASN:HA	1:D:815:ILE:CG1	2.27	0.64
1:B:215:GLY:O	1:B:273:TYR:HB2	1.98	0.64
1:B:395:PHE:CB	1:B:591:GLN:HG2	2.26	0.64
1:C:482:ARG:NE	1:C:556:GLN:HE21	1.91	0.64
1:A:497:GLU:C	1:A:499:ILE:H	2.06	0.64
3:F:108:DT:C2'	3:F:109:DC:H5''	2.28	0.64
1:D:250:VAL:HA	1:D:263:ILE:HD12	1.79	0.63
1:D:52:ILE:HD12	1:D:428:GLU:HG3	1.81	0.63
1:D:784:SER:HA	1:D:829:LYS:HA	1.80	0.63
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.34	0.63
1:B:490:LEU:HA	1:B:493:GLN:HG2	1.81	0.63
1:B:822:PRO:CG	1:B:855:THR:HB	2.28	0.63
1:C:3:GLU:HG2	1:C:21:ASP:HA	1.79	0.63
1:A:23:ASN:HD22	1:A:25:ARG:HH12	1.45	0.63
1:D:124:PRO:HB3	1:D:131:HIS:CD2	2.34	0.63
1:D:874:LYS:HG3	1:D:875:THR:HG23	1.81	0.63
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.80	0.63
1:B:499:ILE:HD12	1:B:530:ILE:HG13	1.81	0.63
1:C:815:ILE:HD12	1:C:821:ALA:HB1	1.80	0.63
1:A:343:LEU:HG	1:A:558:ASN:HD21	1.64	0.62
1:A:362:ILE:HD11	1:A:572:ASN:HB3	1.81	0.62
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.81	0.62
1:D:109:ARG:NH1	1:D:208:LYS:HB3	2.14	0.62
1:D:319:ARG:HG2	1:D:319:ARG:HH11	1.64	0.62
1:D:471:VAL:HG11	1:D:570:LEU:HD11	1.80	0.62
1:A:514:LEU:HD13	1:A:526:ILE:HG23	1.81	0.62
2:G:14:DC:H2''	2:G:15:DC:O5'	1.99	0.62
2:I:6:DA:H2''	2:I:7:DA:H5'	1.81	0.62
1:B:516:VAL:HG11	1:B:526:ILE:CD1	2.29	0.62
1:C:30:GLU:O	1:C:30:GLU:HG2	2.00	0.62
1:D:17:GLU:HG2	1:D:18:ARG:N	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LYS:HD2	1:D:49:TYR:CE2	2.35	0.62
1:D:469:GLY:C	1:D:472:PRO:HD2	2.24	0.62
2:E:6:DA:H2''	2:E:7:DA:C5'	2.29	0.62
1:A:636:VAL:O	1:A:640:LYS:HD2	1.99	0.62
1:A:757:GLU:O	1:A:761:GLN:HG3	1.98	0.62
1:B:197:LEU:HD23	1:B:197:LEU:C	2.24	0.62
1:B:514:LEU:H	1:B:541:MET:CE	2.12	0.62
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.80	0.62
1:D:332:LEU:O	1:D:335:ASP:HB3	1.99	0.62
1:C:544:ARG:HG2	1:C:547:ARG:NH2	2.15	0.62
1:D:645:ASN:O	1:D:649:ASP:HB2	1.99	0.62
1:D:804:HIS:O	1:D:808:ILE:HG13	2.00	0.62
2:I:6:DA:H1'	2:I:7:DA:H5''	1.81	0.62
1:D:109:ARG:NH1	1:D:142:ILE:HD11	2.15	0.62
4:A:982:HOH:O	3:F:114:DA:H5'	2.00	0.62
1:C:149:PHE:O	1:C:197:LEU:HD11	2.00	0.62
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.35	0.62
3:L:104:DG:H2''	3:L:105:DC:H5'	1.81	0.62
1:C:117:VAL:HG22	1:C:133:ILE:HA	1.82	0.62
1:D:90:LEU:CD1	1:D:353:ILE:HG22	2.26	0.62
1:B:231:LYS:HG3	1:B:232:ASN:N	2.14	0.62
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.82	0.62
1:C:179:PRO:HB3	1:C:181:GLU:OE1	1.99	0.62
1:D:833:LEU:HD22	1:D:866:MET:HE3	1.81	0.62
1:B:1:MET:HE1	1:B:20:ILE:CG2	2.30	0.62
1:D:204:PHE:HE1	1:D:208:LYS:HD2	1.65	0.62
1:D:295:GLU:O	1:D:299:ASN:HA	2.00	0.62
1:D:365:TRP:HA	1:D:368:ILE:HD12	1.81	0.62
1:B:339:GLN:OE1	1:B:339:GLN:HA	2.00	0.61
1:C:116:GLU:HG2	1:C:324:ASN:OD1	2.00	0.61
1:C:356:GLN:NE2	1:C:356:GLN:H	1.98	0.61
1:D:269:SER:OG	1:D:355:ILE:HB	1.99	0.61
1:D:356:GLN:OE1	1:D:356:GLN:N	2.33	0.61
1:A:795:GLY:O	1:A:813:ARG:HD3	2.00	0.61
1:D:681:MET:HE2	1:D:681:MET:HA	1.82	0.61
1:D:825:VAL:HG12	1:D:826:GLU:H	1.65	0.61
1:A:494:ARG:HD2	1:A:521:ASP:OD1	1.99	0.61
1:A:555:ALA:O	1:A:559:ARG:HG2	1.99	0.61
1:D:116:GLU:HB3	1:D:320:TYR:OH	2.00	0.61
1:D:202:LEU:O	1:D:206:GLN:HG2	2.01	0.61
1:D:455:SER:HA	1:D:675:ASN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:HIS:HB3	1:D:556:GLN:HB2	1.82	0.61
1:C:313:ARG:HH11	1:C:313:ARG:HG3	1.66	0.61
1:C:486:LYS:HD3	1:C:556:GLN:CD	2.26	0.61
1:A:365:TRP:CD2	1:A:566:LEU:HD23	2.36	0.61
1:B:856:ASP:HA	1:B:859:LYS:CB	2.31	0.61
1:D:542:LEU:HD12	1:D:545:ALA:HB3	1.81	0.61
1:B:900:MET:HE1	1:D:640:LYS:HE3	1.82	0.61
1:C:464:TYR:HB3	1:C:466:ASP:OD2	2.00	0.61
1:A:314:GLU:CG	1:A:315:SER:H	2.14	0.61
1:A:540:GLU:O	1:A:544:ARG:HD3	2.01	0.61
1:B:696:LYS:O	1:B:756:GLY:HA2	2.00	0.61
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.81	0.61
1:C:440:HIS:HD1	1:C:440:HIS:H	1.46	0.61
1:D:439:LEU:O	1:D:443:ILE:HG13	2.01	0.61
1:B:824:VAL:HG13	1:B:830:VAL:HG11	1.81	0.61
1:C:129:ALA:HA	1:C:225:TYR:CZ	2.36	0.61
1:A:855:THR:OG1	1:A:857:LEU:HG	2.00	0.60
1:C:45:GLN:O	1:C:47:THR:HG23	2.01	0.60
1:D:500:LYS:CA	1:D:503:LEU:HB2	2.29	0.60
1:D:732:THR:HG22	1:D:745:LEU:HB3	1.83	0.60
1:D:812:ASN:CA	1:D:815:ILE:HG12	2.28	0.60
1:B:218:VAL:N	1:B:272:ASP:OD2	2.34	0.60
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.35	0.60
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.83	0.60
1:D:493:GLN:HA	1:D:549:GLU:OE1	2.01	0.60
1:D:630:ASP:HB2	4:D:912:HOH:O	2.01	0.60
1:A:85:MET:HE2	1:A:87:ASP:N	2.07	0.60
1:D:15:ILE:HD13	1:D:15:ILE:C	2.26	0.60
1:D:205:TRP:HE1	1:D:242:LEU:CA	2.14	0.60
1:D:243:SER:C	1:D:245:HIS:H	2.09	0.60
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.84	0.60
3:F:111:DT:H2''	3:F:112:DT:H5''	1.83	0.60
1:D:760:LEU:HD23	1:D:760:LEU:C	2.27	0.60
1:A:481:GLN:HE21	1:A:559:ARG:NE	2.00	0.60
1:C:191:PHE:HD2	1:C:196:GLU:HG3	1.66	0.60
1:D:317:HIS:HA	1:D:320:TYR:HB3	1.82	0.60
1:D:511:ASP:OD2	1:D:533:LEU:HA	2.01	0.60
1:D:752:MET:CG	1:D:760:LEU:HD12	2.29	0.60
1:B:556:GLN:HG3	1:B:557:ILE:N	2.17	0.60
1:D:59:ARG:HH11	1:D:59:ARG:HG3	1.66	0.60
1:D:800:LYS:HE3	2:K:13:DG:H4'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:16:DG:C2'	2:G:17:DC:H5''	2.32	0.60
1:A:97:TYR:O	1:A:352:LYS:NZ	2.34	0.60
1:B:278:LYS:HE2	1:B:288:TYR:CD1	2.36	0.60
1:B:338:ARG:O	1:B:339:GLN:HB2	2.02	0.59
1:C:261:GLU:HG3	1:C:261:GLU:O	2.01	0.59
1:C:266:PHE:HD1	1:C:266:PHE:H	1.50	0.59
3:J:104:DG:C2'	3:J:105:DC:H5''	2.32	0.59
1:D:516:VAL:HG21	1:D:522:PHE:CE2	2.37	0.59
1:A:404:TYR:CD1	1:A:618:LEU:HD22	2.37	0.59
1:A:530:ILE:HG23	1:A:541:MET:HE3	1.83	0.59
1:B:355:ILE:O	1:B:358:VAL:HG13	2.02	0.59
1:B:606:ASN:HD22	1:B:612:GLU:CA	2.13	0.59
1:A:792:ASP:HA	1:A:796:PHE:O	2.03	0.59
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.18	0.59
1:D:495:ASN:O	1:D:499:ILE:HG13	2.01	0.59
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.32	0.59
1:D:85:MET:CE	1:D:87:ASP:H	2.15	0.59
1:A:304:LYS:O	1:A:319:ARG:HD3	2.03	0.59
1:B:316:ASN:C	1:B:316:ASN:HD22	2.10	0.59
1:B:554:THR:C	1:B:557:ILE:HG22	2.28	0.59
1:C:449:ARG:HH21	1:C:675:ASN:HB2	1.68	0.59
1:D:802:PRO:HG2	1:D:805:ILE:HG12	1.83	0.59
1:C:323:TYR:HD1	1:C:326:ILE:HD11	1.68	0.59
1:C:482:ARG:HH21	1:C:556:GLN:NE2	2.01	0.59
1:A:23:ASN:ND2	1:A:25:ARG:HH12	2.00	0.59
1:A:791:TYR:CD2	1:A:801:CYS:HA	2.37	0.59
1:B:599:ARG:HG2	1:B:599:ARG:HH11	1.68	0.59
1:B:771:PHE:HD1	1:B:774:LEU:HD12	1.68	0.59
1:D:152:LEU:HA	1:D:159:VAL:HG22	1.83	0.59
2:I:16:DG:H2''	2:I:17:DC:C5'	2.33	0.59
1:A:193:ASN:HB2	4:A:951:HOH:O	2.02	0.59
1:A:731:GLU:H	1:A:731:GLU:CD	2.09	0.59
1:B:114:ASP:HB2	1:B:328:VAL:HG22	1.84	0.59
1:D:812:ASN:HA	1:D:815:ILE:CD1	2.33	0.59
1:B:229:ARG:NH2	1:B:233:ILE:HD11	2.18	0.59
1:D:113:PHE:HB3	1:D:138:HIS:ND1	2.18	0.59
1:B:154:SER:HB2	1:B:155:PRO:HD2	1.84	0.58
1:C:284:ASN:HD21	1:C:829:LYS:HZ1	1.49	0.58
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.02	0.58
1:A:338:ARG:HB3	1:A:340:PHE:CZ	2.38	0.58
1:C:34:LYS:HG3	1:C:63:ALA:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:TYR:O	1:C:281:SER:HB3	2.03	0.58
1:D:228:ASN:O	1:D:231:LYS:HG2	2.02	0.58
1:D:888:LYS:C	1:D:889:LEU:HD12	2.29	0.58
1:A:4:PHE:CE1	1:A:20:ILE:HB	2.38	0.58
1:B:305:TYR:HB2	1:B:312:LEU:HD22	1.85	0.58
1:C:284:ASN:HD21	1:C:829:LYS:NZ	2.00	0.58
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.85	0.58
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.83	0.58
1:C:878:LYS:HE3	4:I:205:HOH:O	2.03	0.58
1:D:205:TRP:HE1	1:D:242:LEU:C	2.10	0.58
1:A:516:VAL:CG1	1:A:526:ILE:HG21	2.34	0.58
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.14	0.58
1:B:815:ILE:CD1	1:B:855:THR:HG21	2.28	0.58
3:J:104:DG:C1'	3:J:105:DC:H5''	2.33	0.58
1:A:248:THR:HG22	1:A:265:LEU:HD23	1.85	0.58
1:A:525:GLU:O	1:A:529:LYS:HE3	2.04	0.58
1:C:11:ILE:HD13	1:C:247:LYS:HD3	1.85	0.58
1:D:474:GLU:OE1	1:D:474:GLU:HA	2.03	0.58
1:D:722:GLU:OE2	1:D:723:PRO:HD2	2.04	0.58
1:A:509:SER:O	1:A:534:SER:HB3	2.03	0.58
1:B:297:GLU:O	1:B:298:LEU:HD23	2.04	0.58
1:B:494:ARG:O	1:B:498:ILE:HG12	2.04	0.58
1:B:776:TYR:CB	1:B:863:LEU:HD13	2.32	0.58
1:C:514:LEU:HG	1:C:533:LEU:HD21	1.85	0.58
1:D:402:ASN:ND2	1:D:403:ARG:N	2.50	0.58
1:B:150:ASP:OD1	1:B:321:ILE:HG13	2.04	0.58
1:B:235:GLY:O	1:B:237:SER:N	2.37	0.58
1:B:642:ARG:NH1	1:B:642:ARG:HB2	2.19	0.58
1:A:653:LYS:HD3	1:A:656:ARG:NH2	2.18	0.58
1:D:365:TRP:CD2	1:D:566:LEU:HD23	2.39	0.58
3:J:110:DA:H2''	3:J:111:DT:H5'	1.86	0.58
1:A:314:GLU:HG3	1:A:315:SER:H	1.68	0.57
1:B:387:PRO:HG2	1:B:389:GLN:NE2	2.12	0.57
1:B:514:LEU:H	1:B:541:MET:HE1	1.68	0.57
1:B:747:GLU:HA	1:B:747:GLU:OE2	2.04	0.57
1:C:231:LYS:HG2	1:C:236:GLU:HA	1.85	0.57
1:D:160:GLU:HG3	1:D:161:GLU:N	2.19	0.57
1:D:732:THR:HG22	1:D:745:LEU:CB	2.34	0.57
1:A:469:GLY:C	1:A:472:PRO:HD2	2.29	0.57
1:B:133:ILE:HD12	1:B:133:ILE:N	2.18	0.57
1:C:291:ASP:O	1:C:295:GLU:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ILE:O	1:C:358:VAL:HG13	2.04	0.57
1:C:461:MET:CE	1:C:581:ARG:HD2	2.34	0.57
1:A:489:MET:HB3	1:A:552:GLY:HA3	1.86	0.57
1:B:227:TYR:CD2	1:B:263:ILE:HD13	2.39	0.57
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.84	0.57
1:C:526:ILE:O	1:C:530:ILE:HG13	2.04	0.57
1:A:101:ILE:HG13	1:A:349:TYR:HB3	1.84	0.57
1:A:481:GLN:HE21	1:A:559:ARG:HE	1.52	0.57
1:C:78:ILE:CG1	1:C:80:LEU:HD23	2.34	0.57
1:D:105:HIS:O	1:D:107:LYS:N	2.37	0.57
1:D:289:SER:O	1:D:293:ILE:HG12	2.05	0.57
1:B:554:THR:CA	1:B:557:ILE:HG22	2.34	0.57
1:C:299:ASN:O	1:C:300:VAL:HG13	2.04	0.57
1:D:118:THR:HB	1:D:313:ARG:NE	2.16	0.57
1:A:412:LEU:HG	1:A:683:MET:HE3	1.87	0.57
1:C:227:TYR:HD2	1:C:228:ASN:ND2	2.02	0.57
2:E:15:DC:H2'	2:E:16:DG:C8	2.39	0.57
1:A:846:ILE:HG23	1:A:846:ILE:O	2.03	0.57
1:B:194:GLU:C	1:B:196:GLU:H	2.12	0.57
1:D:105:HIS:C	1:D:107:LYS:H	2.12	0.57
1:D:147:TYR:CE1	1:D:187:ILE:HD12	2.40	0.57
1:D:395:PHE:HD2	1:D:594:LEU:HD23	1.68	0.57
1:D:728:MET:HG2	3:L:113:DC:H5''	1.87	0.57
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.85	0.57
1:B:792:ASP:OD2	1:B:809:LEU:HD22	2.05	0.57
1:B:836:ARG:NH2	1:B:864:HIS:O	2.38	0.57
1:C:170:LEU:HD22	1:C:170:LEU:N	2.19	0.57
1:C:516:VAL:CG1	1:C:526:ILE:HD13	2.34	0.57
1:A:534:SER:O	1:A:538:LEU:HD12	2.05	0.57
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.85	0.57
1:B:298:LEU:HD13	1:B:333:GLN:HG2	1.86	0.57
1:B:441:ASP:CB	1:B:447:ALA:HB2	2.33	0.57
1:D:40:HIS:CE1	1:D:83:LEU:HD11	2.40	0.57
1:B:188:TYR:OH	1:B:190:PRO:HB3	2.05	0.57
1:D:194:GLU:O	1:D:198:LEU:HD13	2.03	0.57
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.86	0.57
2:E:16:DG:H2''	2:E:17:DC:C5'	2.34	0.57
1:B:660:GLU:HB3	1:B:661:PRO:HD3	1.86	0.56
1:C:815:ILE:HG23	1:C:821:ALA:HB3	1.85	0.56
1:D:671:CYS:SG	1:D:679:HIS:HB2	2.45	0.56
1:B:1:MET:HE1	1:B:20:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PHE:CE1	1:B:208:LYS:HD2	2.40	0.56
1:B:523:SER:H	1:B:526:ILE:HD12	1.71	0.56
1:C:71:TRP:O	1:C:75:MET:HG2	2.05	0.56
1:C:514:LEU:HD12	1:C:530:ILE:HG12	1.86	0.56
1:D:700:GLY:HA2	1:D:753:LEU:CD2	2.36	0.56
1:A:857:LEU:CD1	1:A:858:ILE:HG23	2.30	0.56
1:B:299:ASN:HD22	1:B:299:ASN:N	2.03	0.56
1:C:202:LEU:O	1:C:206:GLN:HG2	2.05	0.56
1:C:227:TYR:HD2	1:C:228:ASN:HD22	1.51	0.56
1:D:573:VAL:HG23	1:D:574:TRP:CD1	2.27	0.56
1:C:81:GLU:HG3	1:C:384:ARG:NH2	2.19	0.56
1:C:154:SER:C	1:C:156:TYR:H	2.14	0.56
1:C:493:GLN:HA	1:C:549:GLU:OE1	2.05	0.56
1:C:529:LYS:O	1:C:529:LYS:HG2	2.06	0.56
1:C:658:ARG:HG2	1:C:658:ARG:HH11	1.70	0.56
1:D:679:HIS:O	1:D:680:LEU:HD23	2.05	0.56
1:D:44:SER:O	1:D:46:ALA:N	2.38	0.56
1:B:771:PHE:HA	1:B:774:LEU:HG	1.87	0.56
1:C:760:LEU:HD13	1:C:891:TYR:HA	1.86	0.56
1:D:513:PRO:HB3	1:D:541:MET:HB2	1.88	0.56
1:A:52:ILE:HD12	1:A:428:GLU:HB3	1.88	0.56
1:B:324:ASN:C	1:B:324:ASN:HD22	2.13	0.56
3:L:104:DG:H1'	3:L:105:DC:H5''	1.88	0.56
1:A:8:VAL:O	1:A:354:GLN:NE2	2.39	0.56
1:C:11:ILE:HD12	1:C:16:PHE:CD2	2.41	0.56
1:C:132:PRO:HB3	1:C:229:ARG:HH21	1.71	0.56
1:C:434:PHE:HE1	1:C:456:CYS:HB3	1.71	0.56
1:D:527:LYS:O	1:D:530:ILE:HG22	2.06	0.56
3:F:104:DG:H2''	3:F:105:DC:H5'	1.86	0.56
1:A:277:TYR:CE2	1:A:293:ILE:HD12	2.41	0.56
1:C:193:ASN:ND2	1:C:195:LYS:HB2	2.20	0.56
1:D:525:GLU:O	1:D:529:LYS:HG3	2.05	0.56
1:D:761:GLN:NE2	1:D:893:LYS:HA	2.20	0.56
1:D:897:LEU:HD12	1:D:898:PHE:N	2.21	0.56
1:B:123:PHE:CD2	1:B:124:PRO:HD2	2.40	0.55
1:B:162:TRP:HZ3	1:B:188:TYR:HB2	1.70	0.55
1:D:274:ILE:O	1:D:278:LYS:HG3	2.05	0.55
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.88	0.55
1:D:534:SER:O	1:D:538:LEU:HG	2.06	0.55
3:F:111:DT:C2'	3:F:112:DT:H5''	2.35	0.55
3:L:103:DG:H2''	3:L:104:DG:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:O	1:A:206:GLN:HG2	2.06	0.55
1:A:687:ALA:HB2	1:A:715:MET:CE	2.35	0.55
1:B:121:ASP:OD1	1:B:122:GLY:N	2.32	0.55
1:C:81:GLU:CD	1:C:384:ARG:HH12	2.14	0.55
1:C:125:GLU:O	1:C:128:GLN:HB2	2.06	0.55
1:C:314:GLU:O	1:C:315:SER:O	2.24	0.55
3:F:104:DG:C1'	3:F:105:DC:H5''	2.33	0.55
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.31	0.55
1:C:477:LYS:O	1:C:481:GLN:HG3	2.06	0.55
1:C:728:MET:CE	3:J:113:DC:H3'	2.36	0.55
1:D:61:LEU:HD13	1:D:62:PHE:N	2.21	0.55
1:B:220:SER:O	1:B:224:PRO:HG2	2.06	0.55
1:B:316:ASN:ND2	1:B:318:GLN:HB3	2.21	0.55
1:B:608:VAL:O	1:B:608:VAL:HG12	2.06	0.55
1:D:71:TRP:CZ2	1:D:75:MET:HE3	2.41	0.55
1:D:664:ASP:O	1:D:668:ARG:HG3	2.06	0.55
1:D:678:GLN:O	1:D:680:LEU:HG	2.06	0.55
1:A:170:LEU:HD12	1:A:173:GLN:HE21	1.72	0.55
1:A:649:ASP:O	1:A:653:LYS:HG2	2.07	0.55
1:B:316:ASN:HD21	1:B:319:ARG:H	1.53	0.55
1:B:542:LEU:O	1:B:546:GLN:HG3	2.07	0.55
1:C:109:ARG:HD2	1:C:209:THR:O	2.07	0.55
1:C:176:ASP:HB2	1:C:178:VAL:HG23	1.88	0.55
1:C:426:SER:OG	1:C:427:PRO:HD2	2.06	0.55
1:B:494:ARG:HD2	1:B:521:ASP:OD1	2.07	0.55
1:C:530:ILE:O	1:C:533:LEU:HB2	2.06	0.55
1:D:145:ARG:NH2	1:D:185:LYS:HG2	2.22	0.55
1:A:785:ALA:HB2	1:A:808:ILE:HD11	1.89	0.55
1:B:186:ILE:HG22	1:B:187:ILE:N	2.22	0.55
1:B:408:MET:CE	1:B:655:ALA:HB2	2.37	0.55
1:B:466:ASP:OD2	1:B:467:ARG:N	2.39	0.55
1:B:487:GLY:HA3	4:B:947:HOH:O	2.05	0.55
1:B:398:GLU:OE1	1:B:705:LYS:HE3	2.05	0.55
1:C:81:GLU:HG3	1:C:384:ARG:HH22	1.71	0.55
1:D:449:ARG:HH21	1:D:675:ASN:CB	2.16	0.55
1:D:118:THR:CB	1:D:313:ARG:HE	2.18	0.55
1:D:541:MET:O	1:D:544:ARG:HB2	2.07	0.55
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.88	0.55
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.89	0.55
1:D:725:LEU:HD11	1:D:750:ARG:HB2	1.88	0.55
1:C:310:SER:C	1:C:312:LEU:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ARG:O	1:B:333:GLN:HB3	2.07	0.54
1:D:248:THR:HA	1:D:266:PHE:CD1	2.42	0.54
1:B:397:LYS:HB3	1:B:620:GLY:H	1.71	0.54
1:D:276:LEU:O	1:D:280:PHE:HD1	1.89	0.54
3:F:111:DT:H1'	3:F:112:DT:H5''	1.89	0.54
1:C:163:SER:OG	1:C:166:ILE:HG13	2.08	0.54
1:C:191:PHE:CE2	1:C:197:LEU:HA	2.43	0.54
1:D:6:LEU:HB2	1:D:18:ARG:O	2.08	0.54
3:F:104:DG:H2''	3:F:105:DC:C5'	2.37	0.54
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.88	0.54
1:D:160:GLU:H	1:D:317:HIS:CD2	2.24	0.54
1:D:819:ILE:O	1:D:819:ILE:HG12	2.07	0.54
1:D:823:GLN:HG2	1:D:824:VAL:O	2.08	0.54
1:A:365:TRP:CE2	1:A:566:LEU:HD23	2.42	0.54
1:A:848:TRP:CE2	1:A:854:ILE:HG12	2.42	0.54
1:B:516:VAL:HG11	1:B:526:ILE:HD11	1.89	0.54
1:C:526:ILE:HG22	1:C:530:ILE:HD11	1.89	0.54
1:D:273:TYR:OH	1:D:340:PHE:HB2	2.07	0.54
1:A:279:LYS:HG3	1:A:280:PHE:CE2	2.43	0.54
1:B:373:LEU:HB3	1:B:378:LYS:HB2	1.89	0.54
1:B:835:LEU:HD21	1:B:846:ILE:HG22	1.89	0.54
1:D:151:LEU:HD23	1:D:151:LEU:C	2.32	0.54
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.89	0.54
1:A:101:ILE:HD11	1:A:349:TYR:O	2.07	0.54
1:A:249:ARG:NH1	1:A:251:LYS:HE2	2.22	0.54
1:B:635:LYS:HG2	1:D:898:PHE:CD2	2.43	0.54
1:C:365:TRP:CE2	1:C:566:LEU:HD23	2.43	0.54
1:C:516:VAL:HG21	1:C:522:PHE:CZ	2.43	0.54
1:D:700:GLY:HA2	1:D:753:LEU:HD22	1.89	0.54
1:D:809:LEU:HA	1:D:812:ASN:OD1	2.07	0.54
1:B:416:TYR:O	1:B:420:ILE:HG13	2.08	0.54
1:C:59:ARG:HG2	1:C:59:ARG:HH11	1.72	0.54
1:C:245:HIS:O	1:C:246:ARG:C	2.51	0.54
1:C:788:ILE:HG13	1:C:826:GLU:OE2	2.07	0.54
1:D:87:ASP:OD1	1:D:363:LYS:HE3	2.08	0.54
1:D:122:GLY:HA3	1:D:823:GLN:HE22	1.73	0.54
1:D:217:ASN:OD1	1:D:220:SER:HB2	2.08	0.54
1:D:594:LEU:O	1:D:597:ILE:HG22	2.08	0.54
1:A:493:GLN:O	1:A:496:GLY:N	2.41	0.54
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.37	0.54
1:B:635:LYS:HG2	1:D:898:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:LEU:O	1:B:813:ARG:HG3	2.08	0.54
1:C:130:LYS:O	1:C:229:ARG:NH1	2.41	0.54
1:C:214:THR:HG23	1:C:215:GLY:N	2.23	0.54
1:C:301:GLY:O	1:C:330:ARG:NH1	2.41	0.54
1:C:415:LEU:CD1	1:C:681:MET:HE1	2.38	0.54
1:A:638:GLU:HB2	4:A:983:HOH:O	2.07	0.54
1:D:18:ARG:HA	1:D:27:ARG:O	2.08	0.54
1:D:298:LEU:C	1:D:300:VAL:H	2.16	0.54
1:D:450:PRO:HB2	1:D:456:CYS:SG	2.49	0.54
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.89	0.53
1:D:19:TYR:O	1:D:26:GLU:HA	2.08	0.53
1:D:25:ARG:HG3	1:D:25:ARG:NH1	2.23	0.53
1:D:146:PHE:N	1:D:146:PHE:CD1	2.75	0.53
1:B:120:PRO:HA	1:B:310:SER:HB3	1.90	0.53
1:A:127:SER:HA	1:A:228:ASN:ND2	2.24	0.53
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.38	0.53
1:B:115:ILE:HD11	1:B:133:ILE:HG13	1.87	0.53
1:B:163:SER:N	1:B:318:GLN:HE22	2.01	0.53
1:C:318:GLN:HE21	1:C:318:GLN:CA	2.19	0.53
1:D:204:PHE:CE1	1:D:208:LYS:HD2	2.44	0.53
3:H:105:DC:H2'	3:H:106:DT:H72	1.89	0.53
3:J:108:DT:H2''	3:J:109:DC:C5'	2.37	0.53
1:B:772:ARG:NH1	1:B:868:TYR:HB3	2.23	0.53
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.26	0.53
1:D:340:PHE:C	1:D:342:ASN:N	2.65	0.53
1:D:362:ILE:HG22	1:D:575:PHE:HD1	1.73	0.53
1:D:771:PHE:HA	1:D:774:LEU:HD12	1.91	0.53
1:A:602:ASN:ND2	1:A:616:PHE:H	2.06	0.53
1:B:824:VAL:CG1	1:B:830:VAL:HG11	2.39	0.53
1:D:9:GLU:HB3	1:D:11:ILE:CD1	2.35	0.53
1:D:50:PHE:HA	1:D:55:LYS:O	2.08	0.53
1:D:61:LEU:HD13	1:D:62:PHE:H	1.73	0.53
1:D:481:GLN:O	1:D:485:HIS:HB2	2.09	0.53
1:B:897:LEU:HD23	1:B:897:LEU:N	2.18	0.53
1:D:206:GLN:NE2	1:D:241:ARG:HB3	2.20	0.53
1:D:830:VAL:HG22	1:D:831:TYR:N	2.24	0.53
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.72	0.53
1:A:620:GLY:HA2	1:A:624:SER:O	2.08	0.53
1:B:198:LEU:O	1:B:200:GLU:N	2.42	0.53
1:B:764:PHE:O	1:B:768:GLU:HG3	2.08	0.53
1:B:835:LEU:HA	1:B:866:MET:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:PRO:HG3	1:D:674:MET:HE2	1.90	0.53
1:D:779:ILE:HD11	1:D:866:MET:HE1	1.90	0.53
1:B:516:VAL:HG11	1:B:526:ILE:HD13	1.91	0.53
1:C:298:LEU:O	1:C:299:ASN:HB2	2.09	0.53
1:C:415:LEU:HD11	1:C:681:MET:HE1	1.90	0.53
1:C:3:GLU:HG2	1:C:21:ASP:C	2.34	0.53
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.38	0.53
1:C:422:GLN:HG3	1:C:678:GLN:O	2.08	0.53
1:D:295:GLU:HG2	1:D:301:GLY:CA	2.28	0.53
1:D:512:GLU:CD	1:D:513:PRO:HD2	2.33	0.53
1:A:280:PHE:CD2	1:A:280:PHE:N	2.74	0.52
1:B:273:TYR:CE2	1:B:335:ASP:HB2	2.44	0.52
1:D:81:GLU:CD	1:D:83:LEU:HD21	2.34	0.52
1:D:433:THR:O	1:D:462:MET:HE2	2.09	0.52
3:J:104:DG:H2''	3:J:105:DC:H5'	1.90	0.52
1:B:700:GLY:HA2	1:B:753:LEU:HD22	1.89	0.52
1:D:150:ASP:OD1	1:D:321:ILE:HG13	2.10	0.52
1:D:516:VAL:HG21	1:D:522:PHE:HZ	1.72	0.52
1:A:261:GLU:C	1:A:262:ILE:HD12	2.34	0.52
1:A:301:GLY:O	1:A:330:ARG:NE	2.36	0.52
1:C:508:LEU:HD23	1:C:508:LEU:C	2.35	0.52
1:A:313:ARG:O	1:A:317:HIS:HB2	2.09	0.52
1:A:784:SER:HB3	1:A:829:LYS:HD3	1.91	0.52
1:B:502:ALA:CB	1:B:530:ILE:HG12	2.34	0.52
1:B:775:ASN:OD1	1:B:776:TYR:N	2.42	0.52
1:C:154:SER:C	1:C:156:TYR:N	2.66	0.52
1:D:513:PRO:CB	1:D:541:MET:HB2	2.39	0.52
1:D:605:LEU:HA	1:D:608:VAL:HG22	1.91	0.52
3:J:101:DG:H2'	3:J:102:DC:C6	2.44	0.52
1:D:19:TYR:CE1	1:D:29:ARG:NE	2.73	0.52
1:B:226:VAL:O	1:B:230:ILE:HG13	2.10	0.52
1:B:334:ILE:CG1	1:B:338:ARG:HG3	2.40	0.52
1:B:340:PHE:O	1:B:343:LEU:HB3	2.09	0.52
1:C:511:ASP:OD2	1:C:533:LEU:HA	2.10	0.52
1:A:422:GLN:HG3	1:A:678:GLN:O	2.10	0.52
1:A:566:LEU:HD13	1:A:566:LEU:C	2.34	0.52
1:B:123:PHE:HE1	1:B:309:ILE:HD11	1.74	0.52
1:D:298:LEU:HB2	1:D:300:VAL:CG1	2.36	0.52
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.91	0.52
1:A:263:ILE:HD12	1:A:263:ILE:N	2.25	0.52
1:B:167:ALA:HB1	1:B:178:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:ND2	1:B:332:LEU:HD23	2.25	0.52
1:B:738:PRO:HB3	1:B:780:ALA:O	2.10	0.52
1:B:805:ILE:HD13	1:B:808:ILE:HD12	1.92	0.52
1:C:313:ARG:HG3	1:C:313:ARG:NH1	2.25	0.52
1:C:474:GLU:OE2	1:C:477:LYS:HD2	2.10	0.52
1:D:698:ILE:HG12	1:D:752:MET:O	2.09	0.52
1:A:731:GLU:HG3	1:A:879:PRO:CB	2.39	0.52
1:B:292:TYR:C	1:B:292:TYR:CD1	2.88	0.52
1:B:524:ASP:C	1:B:526:ILE:H	2.18	0.52
1:C:382:GLN:HB3	1:C:384:ARG:NH1	2.25	0.52
1:D:189:MET:HB3	1:D:191:PHE:CE1	2.45	0.52
1:D:194:GLU:C	1:D:196:GLU:H	2.18	0.52
1:D:399:PRO:HB3	1:D:619:TYR:HD2	1.74	0.52
1:A:290:LEU:O	1:A:294:SER:CB	2.57	0.51
1:B:660:GLU:CB	1:B:661:PRO:HD3	2.40	0.51
1:B:771:PHE:O	1:B:774:LEU:HG	2.10	0.51
1:B:854:ILE:HD11	1:B:858:ILE:CD1	2.40	0.51
1:D:159:VAL:HB	1:D:317:HIS:CD2	2.45	0.51
1:D:197:LEU:HD23	1:D:197:LEU:C	2.35	0.51
1:B:731:GLU:HG3	1:B:879:PRO:HB3	1.92	0.51
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.40	0.51
1:C:134:ASP:O	1:C:135:ALA:HB2	2.10	0.51
1:D:85:MET:HE2	1:D:87:ASP:N	2.23	0.51
1:D:298:LEU:HD11	1:D:333:GLN:HB3	1.91	0.51
1:D:527:LYS:C	1:D:530:ILE:HG22	2.34	0.51
1:D:592:MET:HE3	1:D:670:MET:SD	2.50	0.51
1:B:162:TRP:CZ3	1:B:188:TYR:HB2	2.45	0.51
1:B:376:GLN:HB2	1:B:378:LYS:HG2	1.92	0.51
1:C:787:ASN:HB3	1:C:790:LYS:HB3	1.93	0.51
1:D:250:VAL:HG12	1:D:263:ILE:HD12	1.93	0.51
1:D:402:ASN:HD21	1:D:403:ARG:HG2	1.76	0.51
1:D:423:VAL:O	1:D:424:ASN:HB3	2.10	0.51
1:D:509:SER:H	1:D:534:SER:HB3	1.75	0.51
1:D:757:GLU:O	1:D:761:GLN:HG3	2.11	0.51
1:C:89:LYS:HE3	1:C:354:GLN:OE1	2.10	0.51
1:C:482:ARG:HG3	1:C:556:GLN:HG2	1.91	0.51
1:D:180:SER:O	1:D:183:ILE:HG22	2.10	0.51
1:D:800:LYS:HE3	2:K:13:DG:C4'	2.40	0.51
2:E:8:DT:H2''	2:E:9:DG:C8	2.46	0.51
1:A:401:PRO:O	1:A:402:ASN:HB2	2.11	0.51
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:TYR:CD2	1:A:863:LEU:HD21	2.46	0.51
1:B:198:LEU:O	1:B:199:MET:C	2.53	0.51
1:D:31:VAL:HG21	1:D:92:TYR:OH	2.11	0.51
1:D:38:PHE:HE2	1:D:49:TYR:CG	2.29	0.51
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.75	0.51
1:D:189:MET:HB3	1:D:191:PHE:HE1	1.76	0.51
1:D:251:LYS:HE2	1:D:264:THR:CG2	2.40	0.51
1:D:488:TYR:CE2	1:D:519:ARG:HD2	2.46	0.51
1:D:493:GLN:HA	1:D:549:GLU:CD	2.35	0.51
1:D:849:PRO:HD2	4:D:918:HOH:O	2.11	0.51
3:L:110:DA:H2''	3:L:111:DT:C5'	2.40	0.51
1:B:308:PRO:O	1:B:312:LEU:N	2.43	0.51
1:C:660:GLU:HB3	1:C:661:PRO:HD3	1.92	0.51
1:D:189:MET:CE	1:D:200:GLU:HG2	2.41	0.51
1:D:413:THR:OG1	1:D:682:PHE:HB2	2.10	0.51
1:D:419:ILE:HD13	1:D:589:PHE:HD1	1.75	0.51
3:J:104:DG:H2''	3:J:105:DC:H5''	1.92	0.51
3:J:111:DT:H2'	3:J:112:DT:H71	1.93	0.51
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.92	0.51
1:A:636:VAL:O	1:A:636:VAL:HG12	2.10	0.51
1:B:880:LEU:O	1:B:884:THR:HG23	2.09	0.51
1:C:121:ASP:HA	1:C:819:ILE:HG12	1.93	0.51
1:C:167:ALA:O	1:C:178:VAL:HB	2.11	0.51
1:C:323:TYR:CD1	1:C:326:ILE:HD11	2.46	0.51
1:A:481:GLN:HB3	1:A:559:ARG:HE	1.75	0.51
1:B:513:PRO:HG2	1:B:540:GLU:CG	2.41	0.51
1:B:824:VAL:HG13	1:B:830:VAL:CG1	2.40	0.51
1:D:859:LYS:CG	1:D:860:ASP:H	2.12	0.51
1:A:23:ASN:HD22	1:A:25:ARG:NH1	2.08	0.51
1:A:848:TRP:CD2	1:A:854:ILE:HG12	2.46	0.51
1:B:126:PRO:O	1:B:228:ASN:ND2	2.44	0.51
1:B:873:GLU:HA	1:B:877:ILE:HB	1.92	0.51
1:C:2:LYS:HE2	1:C:102:LYS:HB3	1.91	0.51
1:D:777:ILE:HD11	1:D:853:GLU:OE1	2.11	0.51
2:I:16:DG:H2''	2:I:17:DC:H5'	1.92	0.51
1:A:9:GLU:HA	1:A:89:LYS:HD3	1.93	0.51
1:A:730:LEU:HB3	1:A:883:PHE:CZ	2.46	0.51
1:B:528:GLU:C	1:B:530:ILE:H	2.19	0.51
1:B:546:GLN:O	1:B:550:VAL:HG23	2.11	0.51
1:B:771:PHE:HE2	1:B:872:LEU:HB2	1.76	0.51
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:ASN:HD21	1:C:719:ARG:HH11	1.59	0.51
1:D:731:GLU:HG3	1:D:879:PRO:HB3	1.93	0.51
1:A:728:MET:CE	3:F:113:DC:H3'	2.41	0.50
1:B:134:ASP:OD2	1:B:320:TYR:HE2	1.94	0.50
1:C:580:LEU:C	1:C:580:LEU:HD23	2.36	0.50
1:D:305:TYR:CD2	1:D:312:LEU:HD22	2.46	0.50
1:A:492:ALA:HB1	1:A:549:GLU:HB2	1.92	0.50
1:A:664:ASP:O	1:A:668:ARG:HB2	2.10	0.50
1:B:326:ILE:HG23	1:B:330:ARG:HH21	1.76	0.50
1:C:83:LEU:N	1:C:83:LEU:CD1	2.74	0.50
1:D:248:THR:HA	1:D:266:PHE:HD1	1.76	0.50
1:D:530:ILE:HD11	1:D:541:MET:SD	2.51	0.50
1:A:654:PHE:O	1:A:658:ARG:HB2	2.12	0.50
1:B:282:PHE:O	1:B:283:THR:HG23	2.11	0.50
1:C:458:PRO:HG3	1:C:674:MET:HE2	1.93	0.50
1:D:685:ARG:NH1	1:D:714:ASP:OD2	2.42	0.50
1:A:2:LYS:H	1:A:2:LYS:CD	1.93	0.50
1:A:553:MET:O	1:A:557:ILE:HG12	2.11	0.50
1:A:602:ASN:HD22	1:A:616:PHE:HB2	1.77	0.50
1:B:513:PRO:HG3	1:B:537:SER:O	2.12	0.50
1:D:118:THR:HG22	1:D:313:ARG:NH2	2.26	0.50
1:A:592:MET:HE1	1:A:674:MET:HG3	1.93	0.50
1:B:252:VAL:HG12	1:B:253:ILE:HG13	1.93	0.50
1:C:12:GLY:C	1:C:14:SER:H	2.20	0.50
1:C:203:ASN:N	1:C:203:ASN:HD22	2.09	0.50
1:D:40:HIS:HA	1:D:57:CYS:HB3	1.94	0.50
1:D:214:THR:OG1	1:D:215:GLY:N	2.44	0.50
1:D:344:SER:O	1:D:345:LEU:C	2.54	0.50
3:F:111:DT:H2''	3:F:112:DT:C5'	2.41	0.50
2:G:6:DA:H2''	2:G:7:DA:C5'	2.41	0.50
1:B:188:TYR:CD2	1:B:190:PRO:HD3	2.46	0.50
1:C:500:LYS:HE3	1:C:542:LEU:HD11	1.94	0.50
1:D:360:SER:CB	1:D:363:LYS:HB2	2.41	0.50
1:D:475:ILE:CD1	1:D:563:ILE:HG12	2.42	0.50
1:A:38:PHE:CD2	1:A:59:ARG:HA	2.47	0.50
1:B:298:LEU:O	1:B:299:ASN:HB2	2.11	0.50
1:D:397:LYS:HB3	1:D:620:GLY:H	1.77	0.50
1:A:788:ILE:HD11	1:A:808:ILE:HG21	1.94	0.50
1:B:554:THR:O	1:B:557:ILE:HG22	2.11	0.50
1:C:426:SER:HB3	1:C:428:GLU:OE2	2.12	0.50
1:D:59:ARG:HG3	1:D:59:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:TYR:CG	1:D:140:ASP:N	2.80	0.50
1:D:308:PRO:CG	1:D:311:LYS:HB2	2.36	0.50
1:D:475:ILE:HD11	1:D:563:ILE:HG12	1.92	0.50
1:D:793:VAL:HG23	1:D:796:PHE:HB2	1.94	0.50
2:G:6:DA:H2''	2:G:7:DA:H5'	1.94	0.50
1:C:441:ASP:HB3	1:C:447:ALA:HB2	1.94	0.50
1:D:240:LYS:C	1:D:242:LEU:H	2.20	0.50
1:D:484:GLU:C	1:D:486:LYS:N	2.70	0.50
2:G:13:DG:H1	3:H:105:DC:N4	2.09	0.50
2:I:13:DG:H2''	2:I:14:DC:OP2	2.12	0.50
1:A:491:ALA:C	1:A:493:GLN:H	2.20	0.49
1:B:44:SER:C	1:B:46:ALA:H	2.20	0.49
1:B:800:LYS:HZ1	3:H:108:DT:H5''	1.77	0.49
1:C:404:TYR:CD1	1:C:618:LEU:HD22	2.47	0.49
1:D:202:LEU:O	1:D:205:TRP:HB3	2.12	0.49
1:D:283:THR:HG23	1:D:285:GLN:HE22	1.76	0.49
1:D:298:LEU:C	1:D:300:VAL:N	2.70	0.49
1:D:317:HIS:HA	1:D:320:TYR:CB	2.42	0.49
1:A:202:LEU:CD1	1:A:242:LEU:HD13	2.42	0.49
1:A:281:SER:CB	1:A:338:ARG:HH21	2.22	0.49
1:A:849:PRO:HG2	4:A:933:HOH:O	2.12	0.49
1:C:189:MET:O	1:C:191:PHE:CE1	2.65	0.49
1:C:231:LYS:C	1:C:233:ILE:H	2.20	0.49
3:J:111:DT:C2'	3:J:112:DT:H71	2.42	0.49
1:B:12:GLY:CA	1:B:66:ARG:HH11	2.25	0.49
1:B:830:VAL:HA	1:B:850:SER:HB3	1.94	0.49
1:C:193:ASN:HD22	1:C:195:LYS:HB2	1.78	0.49
1:D:403:ARG:HH21	1:D:698:ILE:HG22	1.77	0.49
1:A:494:ARG:O	1:A:498:ILE:HG12	2.12	0.49
1:B:513:PRO:HB3	1:B:541:MET:HE1	1.94	0.49
1:C:685:ARG:HD2	1:C:685:ARG:C	2.37	0.49
1:D:229:ARG:NH1	1:D:233:ILE:HD11	2.26	0.49
1:D:300:VAL:O	1:D:300:VAL:HG13	2.12	0.49
1:D:305:TYR:HB2	1:D:312:LEU:HD13	1.94	0.49
1:A:508:LEU:HD12	1:A:508:LEU:N	2.28	0.49
1:B:167:ALA:HA	1:B:176:ASP:H	1.76	0.49
1:B:471:VAL:O	1:B:475:ILE:HG22	2.13	0.49
1:B:685:ARG:HD2	1:B:685:ARG:C	2.38	0.49
1:B:898:PHE:C	1:B:900:MET:H	2.21	0.49
1:C:642:ARG:HH11	1:C:646:HIS:CD2	2.30	0.49
1:D:13:ASP:OD2	1:D:66:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TRP:N	1:B:218:VAL:HG13	2.27	0.49
1:B:771:PHE:CD2	1:B:872:LEU:HD13	2.48	0.49
1:B:815:ILE:HG23	1:B:821:ALA:CB	2.43	0.49
1:B:822:PRO:HG2	1:B:855:THR:HB	1.93	0.49
1:C:520:PHE:O	1:C:521:ASP:C	2.55	0.49
1:D:656:ARG:O	1:D:661:PRO:HD3	2.12	0.49
1:D:897:LEU:HD12	1:D:897:LEU:C	2.36	0.49
2:G:16:DG:H2''	2:G:17:DC:H5'	1.93	0.49
1:B:755:GLU:HB3	1:B:759:SER:CB	2.43	0.49
1:D:512:GLU:CG	1:D:513:PRO:HD2	2.42	0.49
1:A:40:HIS:HD2	1:A:57:CYS:SG	2.36	0.49
1:B:123:PHE:CZ	1:B:309:ILE:HD11	2.48	0.49
1:B:133:ILE:CD1	1:B:229:ARG:HG2	2.43	0.49
1:B:738:PRO:HB3	1:B:780:ALA:N	2.27	0.49
1:D:313:ARG:HD3	1:D:320:TYR:CZ	2.47	0.49
1:D:437:ALA:HB3	1:D:442:TYR:CZ	2.47	0.49
1:D:783:SER:O	1:D:830:VAL:N	2.44	0.49
1:A:154:SER:C	1:A:156:TYR:N	2.68	0.49
1:A:170:LEU:HA	1:A:177:GLU:HG2	1.94	0.49
1:A:491:ALA:C	1:A:493:GLN:N	2.67	0.49
1:A:811:TYR:O	1:A:815:ILE:HG12	2.13	0.49
1:B:114:ASP:HB2	1:B:328:VAL:CG2	2.43	0.49
1:B:215:GLY:HA3	1:B:218:VAL:HG11	1.94	0.49
1:D:180:SER:HA	1:D:183:ILE:CG2	2.42	0.49
1:D:294:SER:C	1:D:296:PHE:N	2.70	0.49
1:D:444:ASN:HA	1:D:599:ARG:NE	2.27	0.49
1:D:453:VAL:HG23	1:D:454:TYR:CE2	2.48	0.49
1:A:154:SER:C	1:A:156:TYR:H	2.21	0.49
1:A:369:ILE:HG12	1:A:474:GLU:HG2	1.94	0.49
1:B:490:LEU:C	1:B:492:ALA:H	2.20	0.49
1:B:559:ARG:O	1:B:563:ILE:HG13	2.12	0.49
1:B:606:ASN:ND2	1:B:612:GLU:HA	2.19	0.49
1:B:655:ALA:HA	1:B:659:MET:HB2	1.94	0.49
1:C:13:ASP:HB3	1:C:64:ASN:HB2	1.93	0.49
1:C:481:GLN:HE21	1:C:559:ARG:NE	2.07	0.49
1:C:579:ASP:O	1:C:582:ASN:N	2.46	0.49
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.48	0.49
1:D:9:GLU:O	1:D:11:ILE:HG12	2.12	0.49
1:D:279:LYS:HB3	1:D:280:PHE:CE1	2.48	0.49
1:D:340:PHE:C	1:D:342:ASN:H	2.19	0.49
1:B:11:ILE:HD13	1:B:247:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:TRP:CZ2	1:B:75:MET:HE2	2.48	0.48
1:B:248:THR:HG22	1:B:265:LEU:HA	1.95	0.48
1:C:449:ARG:NH2	1:C:675:ASN:HB2	2.27	0.48
1:D:492:ALA:HB3	1:D:549:GLU:HA	1.95	0.48
1:A:436:VAL:HG12	1:A:437:ALA:O	2.13	0.48
1:B:822:PRO:HB2	1:B:849:PRO:HG2	1.96	0.48
1:C:13:ASP:OD2	1:C:64:ASN:HB2	2.12	0.48
1:D:268:ILE:HG22	1:D:269:SER:N	2.27	0.48
3:H:110:DA:H1'	3:H:111:DT:H5''	1.95	0.48
1:B:472:PRO:HA	1:B:475:ILE:HG22	1.95	0.48
1:B:658:ARG:C	1:B:661:PRO:HD2	2.39	0.48
1:C:846:ILE:HG13	1:C:847:ALA:N	2.27	0.48
1:D:112:ASN:HB3	1:D:214:THR:CG2	2.31	0.48
1:D:126:PRO:HA	1:D:225:TYR:HD1	1.77	0.48
1:D:230:ILE:HG23	1:D:234:PHE:HD2	1.79	0.48
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.96	0.48
1:D:752:MET:HE1	1:D:884:THR:HA	1.95	0.48
1:A:21:ASP:OD2	1:A:21:ASP:C	2.57	0.48
1:A:454:TYR:HB3	1:A:463:TYR:O	2.13	0.48
1:B:830:VAL:CA	1:B:850:SER:HB3	2.43	0.48
1:C:109:ARG:CZ	1:C:142:ILE:HD12	2.43	0.48
1:C:197:LEU:HD23	1:C:197:LEU:C	2.37	0.48
1:D:305:TYR:O	1:D:307:GLY:N	2.46	0.48
3:J:113:DC:C2'	3:J:114:DA:H5''	2.36	0.48
1:A:546:GLN:O	1:A:547:ARG:C	2.56	0.48
1:B:38:PHE:CE2	1:B:59:ARG:HB2	2.48	0.48
1:B:159:VAL:HG11	1:B:313:ARG:HG2	1.95	0.48
1:C:130:LYS:CG	1:C:131:HIS:H	2.13	0.48
1:D:93:LEU:HD12	1:D:352:LYS:O	2.12	0.48
1:C:6:LEU:HD13	1:C:211:VAL:HG21	1.95	0.48
1:D:31:VAL:CG1	1:D:32:GLU:N	2.75	0.48
1:D:434:PHE:CZ	1:D:460:GLY:HA2	2.48	0.48
1:D:512:GLU:HG3	1:D:513:PRO:HD2	1.95	0.48
1:D:599:ARG:HG2	1:D:599:ARG:HH11	1.78	0.48
1:D:698:ILE:O	1:D:753:LEU:O	2.31	0.48
1:D:705:LYS:C	1:D:707:ARG:H	2.21	0.48
1:C:642:ARG:HD2	1:C:646:HIS:CE1	2.48	0.48
1:D:813:ARG:NH2	1:D:842:GLY:HA3	2.29	0.48
3:L:104:DG:H2''	3:L:105:DC:C5'	2.42	0.48
1:A:87:ASP:OD1	1:A:363:LYS:NZ	2.43	0.48
1:A:405:LYS:HG2	1:A:406:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:HA	1:B:319:ARG:HH21	1.78	0.48
1:B:302:LYS:HG2	1:B:303:LEU:H	1.79	0.48
1:B:456:CYS:SG	1:B:462:MET:HG2	2.53	0.48
1:C:51:ASP:HB2	4:C:919:HOH:O	2.14	0.48
1:C:170:LEU:HD22	1:C:170:LEU:H	1.79	0.48
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.49	0.48
1:D:10:GLN:HG3	1:D:65:MET:HE1	1.94	0.48
1:D:31:VAL:CG1	1:D:32:GLU:H	2.23	0.48
1:D:305:TYR:C	1:D:307:GLY:H	2.22	0.48
1:D:368:ILE:HG22	1:D:474:GLU:OE2	2.12	0.48
1:A:11:ILE:HD12	1:A:16:PHE:CD1	2.49	0.48
1:A:850:SER:O	1:A:852:THR:HG23	2.13	0.48
1:B:217:ASN:HB2	1:B:274:ILE:CD1	2.40	0.48
1:D:28:THR:HG22	1:D:29:ARG:N	2.29	0.48
1:D:596:TRP:CZ2	1:D:670:MET:HB2	2.48	0.48
2:E:16:DG:H1'	2:E:17:DC:H5''	1.95	0.48
1:A:86:ASP:OD1	1:A:86:ASP:N	2.44	0.48
1:A:152:LEU:HB2	1:A:191:PHE:O	2.14	0.48
1:A:170:LEU:CG	1:A:173:GLN:HE21	2.26	0.48
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.49	0.48
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.48	0.48
1:A:752:MET:CG	1:A:760:LEU:HD22	2.43	0.48
1:B:776:TYR:N	4:B:916:HOH:O	2.46	0.48
1:C:121:ASP:OD2	1:C:131:HIS:NE2	2.47	0.48
1:D:6:LEU:HD11	1:D:26:GLU:HG2	1.95	0.48
1:D:295:GLU:CD	1:D:301:GLY:HA2	2.38	0.48
1:B:316:ASN:ND2	1:B:316:ASN:C	2.71	0.47
1:B:439:LEU:O	1:B:443:ILE:HG13	2.14	0.47
1:C:137:THR:OG1	1:C:324:ASN:ND2	2.47	0.47
1:C:455:SER:HA	1:C:675:ASN:O	2.13	0.47
1:D:205:TRP:CZ3	1:D:210:PRO:HG2	2.49	0.47
1:D:226:VAL:O	1:D:230:ILE:HG13	2.14	0.47
1:D:881:GLU:O	1:D:882:GLY:C	2.57	0.47
1:A:126:PRO:HB3	1:A:224:PRO:HB2	1.96	0.47
1:A:731:GLU:CD	1:A:731:GLU:N	2.71	0.47
1:B:500:LYS:HA	1:B:503:LEU:HB2	1.95	0.47
1:B:708:TYR:CZ	1:B:728:MET:HG3	2.50	0.47
1:B:775:ASN:O	1:B:779:ILE:HG12	2.14	0.47
1:B:799:PRO:O	1:B:800:LYS:C	2.57	0.47
1:C:496:GLY:O	1:C:500:LYS:HG2	2.14	0.47
1:B:178:VAL:O	1:B:179:PRO:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:CD2	1:B:197:LEU:HA	2.49	0.47
1:B:737:THR:CG2	1:B:738:PRO:HD2	2.45	0.47
1:C:11:ILE:CD1	1:C:247:LYS:HD3	2.43	0.47
1:C:343:LEU:HD11	1:C:558:ASN:ND2	2.30	0.47
1:D:151:LEU:HD21	1:D:154:SER:OG	2.14	0.47
1:D:673:TYR:C	1:D:675:ASN:H	2.20	0.47
3:H:103:DG:H2''	3:H:104:DG:OP2	2.14	0.47
1:A:206:GLN:NE2	1:A:246:ARG:HH22	2.11	0.47
1:A:303:LEU:HB3	1:A:323:TYR:HD1	1.80	0.47
1:C:313:ARG:O	1:C:317:HIS:HB2	2.15	0.47
1:C:439:LEU:HD11	1:C:592:MET:HB2	1.97	0.47
1:D:131:HIS:C	1:D:229:ARG:HE	2.23	0.47
1:D:276:LEU:O	1:D:280:PHE:CD1	2.66	0.47
1:A:598:GLU:HG3	1:A:617:VAL:HG11	1.95	0.47
1:B:197:LEU:HD22	1:B:198:LEU:HD23	1.97	0.47
1:C:51:ASP:C	1:C:51:ASP:OD1	2.57	0.47
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.25	0.47
1:D:411:ASP:HA	1:D:623:ASP:O	2.14	0.47
3:H:104:DG:H1'	3:H:105:DC:H5''	1.95	0.47
1:B:499:ILE:HA	1:B:530:ILE:HD11	1.95	0.47
1:C:111:ALA:HB2	1:C:210:PRO:HB3	1.96	0.47
1:C:176:ASP:O	1:C:178:VAL:N	2.41	0.47
1:C:330:ARG:O	1:C:334:ILE:HG13	2.15	0.47
1:C:818:ASN:HD22	1:C:821:ALA:N	2.11	0.47
1:D:7:THR:O	1:D:17:GLU:HA	2.13	0.47
1:D:40:HIS:HE1	1:D:83:LEU:HD11	1.80	0.47
1:D:138:HIS:HD2	1:D:204:PHE:CE2	2.33	0.47
1:D:205:TRP:CD1	1:D:242:LEU:HA	2.49	0.47
1:D:230:ILE:C	1:D:232:ASN:H	2.21	0.47
1:D:244:PRO:HG2	1:D:267:GLY:HA3	1.97	0.47
1:D:449:ARG:O	1:D:450:PRO:C	2.58	0.47
1:D:516:VAL:CG1	1:D:526:ILE:HG21	2.30	0.47
1:D:579:ASP:C	1:D:579:ASP:OD2	2.57	0.47
2:E:16:DG:H2''	2:E:17:DC:H5'	1.96	0.47
1:A:362:ILE:HG22	1:A:363:LYS:N	2.30	0.47
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.45	0.47
1:A:481:GLN:NE2	1:A:559:ARG:NE	2.61	0.47
1:B:136:ILE:HD11	1:B:201:TYR:CE1	2.50	0.47
1:B:222:ALA:O	1:B:226:VAL:HG23	2.15	0.47
1:B:234:PHE:N	1:B:234:PHE:CD1	2.83	0.47
1:B:240:LYS:C	1:B:242:LEU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:PRO:HB3	1:B:780:ALA:C	2.40	0.47
1:B:804:HIS:CE1	1:B:805:ILE:HG12	2.50	0.47
1:C:151:LEU:HD21	1:C:153:ASN:O	2.15	0.47
1:C:180:SER:C	1:C:182:ILE:H	2.22	0.47
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.96	0.47
1:C:604:TYR:OH	1:C:658:ARG:HB3	2.15	0.47
1:C:818:ASN:HD21	1:C:820:ASP:HB2	1.80	0.47
1:D:28:THR:O	1:D:29:ARG:HB3	2.15	0.47
1:D:294:SER:O	1:D:296:PHE:N	2.47	0.47
1:D:591:GLN:HG2	1:D:595:GLN:NE2	2.29	0.47
2:G:17:DC:H2''	2:G:18:DG:O5'	2.15	0.47
3:J:101:DG:H2'	3:J:102:DC:C5	2.50	0.47
1:C:17:GLU:HG2	1:C:18:ARG:N	2.28	0.47
1:C:529:LYS:O	1:C:533:LEU:HD13	2.15	0.47
1:D:119:SER:OG	1:D:124:PRO:HD3	2.14	0.47
1:A:170:LEU:CD1	1:A:173:GLN:HE21	2.27	0.47
1:A:360:SER:HB3	1:A:363:LYS:HB3	1.97	0.47
1:B:159:VAL:HG11	1:B:313:ARG:CG	2.44	0.47
1:B:268:ILE:HG22	1:B:269:SER:N	2.30	0.47
1:B:554:THR:HA	1:B:557:ILE:HG21	1.97	0.47
1:B:606:ASN:ND2	1:B:613:GLY:N	2.62	0.47
1:B:807:GLY:HA2	1:B:845:CYS:O	2.15	0.47
1:C:151:LEU:HD23	1:C:152:LEU:N	2.30	0.47
1:C:424:ASN:HD22	1:C:472:PRO:HG2	1.80	0.47
1:D:4:PHE:CE2	1:D:20:ILE:HG21	2.49	0.47
1:D:109:ARG:CZ	1:D:208:LYS:HB3	2.45	0.47
1:D:111:ALA:HB1	1:D:139:TYR:O	2.15	0.47
1:D:162:TRP:HB3	1:D:188:TYR:CZ	2.50	0.47
1:D:289:SER:O	1:D:290:LEU:C	2.57	0.47
1:D:642:ARG:HH11	1:D:642:ARG:HG3	1.80	0.47
1:A:148:VAL:HG21	1:A:325:ILE:HD11	1.97	0.47
1:A:182:ILE:HG21	1:A:329:TYR:CE1	2.49	0.47
1:A:279:LYS:CG	1:A:280:PHE:CE2	2.97	0.47
1:A:285:GLN:HB3	1:A:292:TYR:HE2	1.79	0.47
1:A:403:ARG:HD2	1:A:887:ALA:O	2.15	0.47
1:A:414:SER:O	1:A:417:PRO:HD2	2.15	0.47
1:C:13:ASP:OD2	1:C:66:ARG:HB3	2.15	0.47
1:C:151:LEU:CD2	1:C:153:ASN:H	2.28	0.47
1:C:213:LEU:HD13	1:C:223:ILE:HD11	1.96	0.47
1:C:318:GLN:CA	1:C:318:GLN:NE2	2.78	0.47
1:D:286:PRO:O	1:D:829:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:PRO:O	1:D:508:LEU:HD22	2.14	0.47
1:A:787:ASN:HD22	1:A:790:LYS:HE2	1.78	0.46
1:B:235:GLY:O	1:B:236:GLU:C	2.58	0.46
1:B:725:LEU:HD22	1:B:753:LEU:HD12	1.96	0.46
1:C:59:ARG:HG2	1:C:59:ARG:NH1	2.30	0.46
1:C:154:SER:O	1:C:156:TYR:N	2.48	0.46
1:C:503:LEU:HG	1:C:538:LEU:HB3	1.97	0.46
1:C:578:TYR:OH	1:C:580:LEU:HB2	2.15	0.46
1:D:433:THR:CG2	1:D:461:MET:HE3	2.44	0.46
1:D:516:VAL:HG12	1:D:526:ILE:HD13	1.97	0.46
1:A:117:VAL:O	1:A:117:VAL:HG12	2.14	0.46
1:A:671:CYS:SG	1:A:676:ASN:HB2	2.55	0.46
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.29	0.46
1:B:642:ARG:HB2	1:B:642:ARG:HH11	1.80	0.46
1:B:801:CYS:O	1:B:802:PRO:O	2.33	0.46
1:C:481:GLN:O	1:C:484:GLU:HB3	2.15	0.46
1:D:685:ARG:HD2	1:D:685:ARG:C	2.40	0.46
1:D:687:ALA:HB2	1:D:715:MET:HE1	1.96	0.46
3:F:110:DA:H1'	3:F:111:DT:H5''	1.97	0.46
1:A:507:ASN:C	1:A:508:LEU:HD12	2.40	0.46
1:B:229:ARG:HE	1:B:233:ILE:HD11	1.78	0.46
1:B:755:GLU:HG2	1:B:759:SER:OG	2.15	0.46
1:C:530:ILE:HA	1:C:533:LEU:HD13	1.97	0.46
1:D:206:GLN:HE22	1:D:241:ARG:CB	2.22	0.46
1:D:345:LEU:HA	1:D:355:ILE:HD12	1.97	0.46
1:D:543:PHE:CA	1:D:546:GLN:HE21	2.08	0.46
3:H:107:DG:H2''	3:H:108:DT:OP2	2.14	0.46
1:B:499:ILE:HA	1:B:530:ILE:CD1	2.46	0.46
1:D:652:ASP:OD2	1:D:652:ASP:C	2.58	0.46
1:D:735:SER:O	1:D:782:VAL:HB	2.15	0.46
3:L:108:DT:H1'	3:L:109:DC:H5''	1.97	0.46
1:A:85:MET:HE3	1:A:85:MET:CA	2.46	0.46
1:A:214:THR:HG21	1:A:341:ILE:HD11	1.97	0.46
1:B:150:ASP:OD2	1:B:151:LEU:N	2.49	0.46
1:B:364:THR:HG21	1:B:562:LEU:HD11	1.97	0.46
1:B:458:PRO:HG3	1:B:592:MET:SD	2.56	0.46
1:B:489:MET:SD	1:B:553:MET:HG2	2.55	0.46
1:C:450:PRO:HB2	1:C:456:CYS:SG	2.55	0.46
1:C:596:TRP:HZ2	1:C:669:GLU:HG2	1.80	0.46
1:D:68:ALA:O	1:D:72:ILE:HG13	2.16	0.46
1:D:143:ASP:HB3	1:D:147:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:VAL:HG23	1:D:793:VAL:O	2.15	0.46
1:A:165:GLU:H	1:A:165:GLU:CD	2.22	0.46
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.96	0.46
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.97	0.46
1:B:133:ILE:HD12	1:B:133:ILE:H	1.81	0.46
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.50	0.46
1:B:804:HIS:NE2	1:B:805:ILE:HG12	2.30	0.46
1:B:862:VAL:O	1:B:862:VAL:HG22	2.15	0.46
1:D:347:MET:SD	1:D:562:LEU:HD11	2.56	0.46
1:D:747:GLU:O	1:D:751:ARG:HG3	2.15	0.46
1:A:6:LEU:HD11	1:A:20:ILE:CD1	2.46	0.46
1:A:426:SER:HB3	1:A:429:THR:HG23	1.98	0.46
1:A:470:VAL:O	1:A:474:GLU:HB2	2.15	0.46
1:A:492:ALA:CB	1:A:549:GLU:HB2	2.45	0.46
1:A:653:LYS:O	1:A:657:GLU:HG2	2.16	0.46
1:B:1:MET:HE1	1:B:20:ILE:HG21	1.98	0.46
1:B:121:ASP:CG	1:B:122:GLY:H	2.17	0.46
1:B:739:LYS:O	1:B:740:ALA:C	2.59	0.46
1:C:760:LEU:C	1:C:760:LEU:HD22	2.40	0.46
1:D:1:MET:HE3	1:D:102:LYS:CE	2.43	0.46
1:D:159:VAL:HB	1:D:317:HIS:CG	2.51	0.46
1:D:556:GLN:O	1:D:556:GLN:NE2	2.48	0.46
1:D:641:PHE:CG	1:D:647:TRP:HB3	2.51	0.46
1:D:799:PRO:O	1:D:800:LYS:HB2	2.16	0.46
1:D:812:ASN:C	1:D:815:ILE:HG12	2.41	0.46
1:B:313:ARG:O	1:B:317:HIS:HB2	2.16	0.46
1:C:413:THR:O	1:C:414:SER:C	2.58	0.46
1:C:738:PRO:HG2	1:C:741:VAL:HB	1.98	0.46
1:C:818:ASN:ND2	1:C:821:ALA:H	2.11	0.46
2:G:12:DA:H61	3:H:106:DT:H3	1.64	0.46
1:A:482:ARG:CZ	1:A:556:GLN:HE21	2.28	0.46
1:B:115:ILE:CD1	1:B:133:ILE:HG12	2.43	0.46
1:B:295:GLU:O	1:B:299:ASN:HA	2.16	0.46
1:C:125:GLU:CD	1:C:126:PRO:HD2	2.40	0.46
1:D:140:ASP:OD1	1:D:142:ILE:HG12	2.15	0.46
1:D:652:ASP:OD2	1:D:656:ARG:NH1	2.49	0.46
1:D:776:TYR:CD2	1:D:863:LEU:HD11	2.51	0.46
2:G:16:DG:H1'	2:G:17:DC:H5''	1.98	0.46
1:A:50:PHE:HD2	1:A:54:GLY:O	1.99	0.46
1:A:516:VAL:HG13	1:A:526:ILE:HG21	1.98	0.46
1:B:194:GLU:C	1:B:196:GLU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:HG22	1:B:265:LEU:HD23	1.97	0.46
1:C:170:LEU:HD12	1:C:177:GLU:OE2	2.16	0.46
1:C:178:VAL:O	1:C:179:PRO:C	2.58	0.46
1:D:630:ASP:O	1:D:632:ILE:N	2.49	0.46
2:I:4:CTG:H2''	2:I:5:DG:OP2	2.16	0.46
1:A:808:ILE:HD13	1:A:824:VAL:HG11	1.98	0.45
1:B:308:PRO:C	1:B:310:SER:H	2.24	0.45
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.97	0.45
1:B:592:MET:HE3	1:B:670:MET:SD	2.56	0.45
1:B:609:CYS:C	1:B:611:THR:N	2.74	0.45
1:B:808:ILE:HG23	1:B:824:VAL:HG21	1.98	0.45
1:B:834:PRO:O	1:B:866:MET:HA	2.16	0.45
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.46	0.45
1:C:482:ARG:HH21	1:C:556:GLN:HE22	1.63	0.45
1:D:51:ASP:C	1:D:51:ASP:OD2	2.58	0.45
1:D:137:THR:HG22	1:D:328:VAL:HG21	1.98	0.45
1:D:316:ASN:ND2	1:D:319:ARG:CB	2.78	0.45
1:D:830:VAL:HG23	1:D:848:TRP:C	2.41	0.45
2:I:16:DG:H2''	2:I:17:DC:H5''	1.98	0.45
1:A:420:ILE:HG12	1:A:586:ILE:HD11	1.99	0.45
1:B:815:ILE:HG23	1:B:821:ALA:HB3	1.98	0.45
1:D:500:LYS:C	1:D:503:LEU:H	2.25	0.45
1:D:831:TYR:CD2	1:D:848:TRP:NE1	2.74	0.45
3:H:104:DG:H5''	4:H:161:HOH:O	2.15	0.45
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.51	0.45
1:A:788:ILE:CD1	1:A:808:ILE:HG21	2.46	0.45
1:B:200:GLU:O	1:B:204:PHE:N	2.46	0.45
1:C:317:HIS:O	1:C:318:GLN:C	2.60	0.45
1:C:426:SER:CB	1:C:428:GLU:OE2	2.65	0.45
1:C:647:TRP:CE3	1:C:651:LEU:HD12	2.51	0.45
1:D:38:PHE:CZ	1:D:59:ARG:HG2	2.51	0.45
1:D:344:SER:O	1:D:347:MET:N	2.49	0.45
1:D:351:ALA:HB3	1:D:353:ILE:HG12	1.98	0.45
1:D:514:LEU:N	1:D:541:MET:HE2	2.31	0.45
1:D:687:ALA:HB2	1:D:715:MET:CE	2.46	0.45
1:D:789:ALA:O	1:D:792:ASP:HB3	2.17	0.45
1:D:793:VAL:C	1:D:795:GLY:H	2.24	0.45
1:D:813:ARG:HH22	1:D:843:ASP:H	1.64	0.45
3:H:104:DG:H2''	3:H:105:DC:H5'	1.96	0.45
1:A:283:THR:O	1:A:284:ASN:C	2.60	0.45
1:B:391:TYR:HB2	1:B:392:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASP:C	1:C:178:VAL:H	2.23	0.45
1:C:286:PRO:HD2	1:C:292:TYR:CE1	2.51	0.45
1:C:451:SER:OG	1:C:452:ASP:N	2.49	0.45
1:C:526:ILE:HG22	1:C:530:ILE:CD1	2.45	0.45
1:D:7:THR:HG21	1:D:18:ARG:HE	1.81	0.45
1:D:62:PHE:N	1:D:62:PHE:CD1	2.84	0.45
1:D:736:SER:HA	1:D:782:VAL:O	2.16	0.45
3:H:111:DT:H2''	3:H:112:DT:OP2	2.17	0.45
1:A:371:ASN:O	1:A:375:GLU:HG2	2.16	0.45
1:B:115:ILE:HG13	1:B:133:ILE:HG21	1.99	0.45
1:B:324:ASN:C	1:B:324:ASN:ND2	2.72	0.45
1:B:408:MET:SD	1:B:655:ALA:HB2	2.56	0.45
1:B:658:ARG:O	1:B:661:PRO:HD2	2.17	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.99	0.45
1:D:148:VAL:HG21	1:D:325:ILE:CD1	2.47	0.45
1:D:224:PRO:O	1:D:228:ASN:ND2	2.50	0.45
1:D:396:VAL:HG12	1:D:705:LYS:HD3	1.98	0.45
1:D:740:ALA:O	1:D:741:VAL:C	2.59	0.45
1:D:822:PRO:HB2	1:D:849:PRO:HG2	1.98	0.45
3:L:108:DT:C1'	3:L:109:DC:H5''	2.46	0.45
1:C:844:LYS:HZ1	2:I:12:DA:P	2.40	0.45
1:D:793:VAL:CG2	1:D:796:PHE:HB2	2.47	0.45
1:D:880:LEU:O	1:D:884:THR:HG23	2.17	0.45
1:B:333:GLN:O	1:B:336:ALA:HB3	2.15	0.45
1:C:13:ASP:CG	1:C:64:ASN:HB2	2.42	0.45
1:C:116:GLU:HB3	1:C:320:TYR:OH	2.16	0.45
1:C:233:ILE:HG22	1:C:234:PHE:N	2.31	0.45
1:D:151:LEU:HD11	1:D:154:SER:OG	2.17	0.45
1:D:251:LYS:HE2	1:D:264:THR:HG21	1.97	0.45
3:J:105:DC:H2'	3:J:106:DT:H72	1.98	0.45
1:B:272:ASP:CG	1:B:274:ILE:HG22	2.42	0.45
1:B:415:LEU:CD1	1:B:681:MET:HE1	2.47	0.45
1:B:529:LYS:O	1:B:533:LEU:HG	2.15	0.45
1:B:589:PHE:CD1	1:B:589:PHE:C	2.94	0.45
1:C:153:ASN:HB2	1:C:192:ASP:O	2.17	0.45
1:C:300:VAL:HG23	1:C:300:VAL:O	2.17	0.45
1:D:243:SER:C	1:D:245:HIS:N	2.75	0.45
1:D:285:GLN:C	1:D:287:SER:N	2.72	0.45
1:D:285:GLN:HB3	1:D:292:TYR:CE2	2.52	0.45
1:D:365:TRP:O	1:D:369:ILE:HG13	2.17	0.45
1:D:367:ALA:O	1:D:370:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:PHE:CZ	1:D:397:LYS:HB2	2.52	0.45
1:D:800:LYS:H	2:K:13:DG:H5''	1.82	0.45
1:A:405:LYS:O	1:A:690:GLY:HA2	2.17	0.45
1:A:490:LEU:O	1:A:493:GLN:HB2	2.16	0.45
1:A:833:LEU:HD22	1:A:866:MET:HE3	1.98	0.45
1:B:36:SER:O	1:B:37:LEU:HD13	2.17	0.45
1:C:234:PHE:HB3	1:C:238:THR:HG21	1.99	0.45
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.65	0.45
1:A:214:THR:OG1	1:A:215:GLY:N	2.50	0.45
1:B:134:ASP:OD2	1:B:320:TYR:CE2	2.70	0.45
1:B:312:LEU:HD23	1:B:320:TYR:HD1	1.81	0.45
1:B:606:ASN:ND2	1:B:612:GLU:CA	2.78	0.45
1:B:696:LYS:O	1:B:756:GLY:CA	2.64	0.45
1:B:751:ARG:CZ	1:B:763:TYR:HB2	2.47	0.45
1:C:457:SER:C	1:C:459:ASN:H	2.25	0.45
1:D:7:THR:CG2	1:D:18:ARG:HG3	2.47	0.45
1:D:114:ASP:HB3	1:D:328:VAL:HG12	1.98	0.45
1:D:212:ILE:HD13	1:D:269:SER:HB3	1.98	0.45
1:D:248:THR:CG2	1:D:249:ARG:N	2.79	0.45
2:E:7:DA:H5'	4:E:19:HOH:O	2.16	0.45
2:G:12:DA:C2	3:H:107:DG:C2	3.05	0.45
2:K:9:DG:H2''	2:K:10:DA:OP2	2.15	0.45
2:K:15:DC:C2'	2:K:16:DG:C8	2.90	0.45
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.98	0.44
1:A:542:LEU:C	1:A:542:LEU:HD12	2.42	0.44
1:A:816:LYS:HD2	1:A:816:LYS:C	2.42	0.44
1:A:840:PRO:HD3	1:A:865:TRP:CE2	2.53	0.44
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.85	0.44
1:B:198:LEU:C	1:B:200:GLU:N	2.74	0.44
1:C:52:ILE:HG12	4:C:919:HOH:O	2.16	0.44
1:D:17:GLU:HG2	1:D:18:ARG:H	1.82	0.44
1:D:402:ASN:HD22	1:D:403:ARG:N	2.13	0.44
1:D:856:ASP:HA	1:D:859:LYS:HD2	1.99	0.44
2:K:13:DG:H2''	2:K:14:DC:OP2	2.17	0.44
1:A:189:MET:O	1:A:191:PHE:CE1	2.71	0.44
1:A:299:ASN:O	1:A:300:VAL:HG13	2.17	0.44
1:A:481:GLN:NE2	1:A:559:ARG:HE	2.14	0.44
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.52	0.44
1:B:271:LEU:CD1	1:B:356:GLN:HA	2.46	0.44
1:B:502:ALA:HB3	1:B:530:ILE:CG1	2.39	0.44
1:B:609:CYS:C	1:B:611:THR:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:808:ILE:O	1:B:808:ILE:HG22	2.16	0.44
1:B:831:TYR:CD2	1:B:850:SER:HA	2.51	0.44
1:C:45:GLN:O	1:C:46:ALA:C	2.59	0.44
1:C:405:LYS:O	1:C:690:GLY:HA2	2.17	0.44
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.88	0.44
1:D:137:THR:N	1:D:324:ASN:ND2	2.63	0.44
1:D:422:GLN:O	1:D:676:ASN:HB3	2.17	0.44
1:D:455:SER:OG	1:D:676:ASN:HA	2.16	0.44
1:D:503:LEU:HG	1:D:538:LEU:HD13	1.99	0.44
1:D:514:LEU:HD12	1:D:530:ILE:HB	1.99	0.44
1:A:745:LEU:HD13	1:A:876:PHE:HD1	1.82	0.44
1:B:775:ASN:HB3	1:B:778:SER:OG	2.17	0.44
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.32	0.44
1:C:126:PRO:C	1:C:128:GLN:H	2.26	0.44
1:C:426:SER:OG	1:C:428:GLU:OE2	2.34	0.44
1:D:484:GLU:C	1:D:486:LYS:H	2.24	0.44
1:D:809:LEU:C	1:D:809:LEU:HD12	2.42	0.44
1:A:227:TYR:CD2	1:A:263:ILE:HG12	2.52	0.44
1:B:114:ASP:HB3	1:B:324:ASN:HD21	1.83	0.44
1:C:702:TRP:CZ3	1:C:710:LEU:HD21	2.53	0.44
1:D:85:MET:HE1	1:D:576:ARG:NH2	2.33	0.44
1:D:459:ASN:OD1	1:D:584:THR:HG22	2.17	0.44
1:D:497:GLU:O	1:D:498:ILE:HD13	2.18	0.44
1:D:692:PRO:HG3	1:D:713:TRP:HZ2	1.82	0.44
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.33	0.44
1:D:788:ILE:HD11	1:D:825:VAL:O	2.17	0.44
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.99	0.44
1:B:608:VAL:HG11	1:D:897:LEU:HD21	2.00	0.44
1:C:178:VAL:CG2	1:C:322:SER:HB3	2.48	0.44
1:C:265:LEU:O	1:C:266:PHE:C	2.59	0.44
1:C:434:PHE:C	1:C:434:PHE:CD2	2.96	0.44
1:C:557:ILE:HD13	1:C:557:ILE:HA	1.84	0.44
2:K:11:DC:H2"	2:K:12:DA:C8	2.52	0.44
1:A:225:TYR:O	1:A:226:VAL:C	2.60	0.44
1:A:605:LEU:O	1:A:609:CYS:HB2	2.18	0.44
1:B:13:ASP:OD1	1:B:66:ARG:HB2	2.18	0.44
1:B:246:ARG:HH11	1:B:246:ARG:HG3	1.82	0.44
1:B:855:THR:HG23	1:B:858:ILE:HG12	2.00	0.44
1:C:530:ILE:HG23	1:C:533:LEU:HD22	2.00	0.44
1:C:546:GLN:C	1:C:548:THR:N	2.74	0.44
1:D:105:HIS:C	1:D:107:LYS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.99	0.44
3:H:109:DC:H2''	3:H:110:DA:O5'	2.16	0.44
1:A:777:ILE:HG23	1:A:831:TYR:CE2	2.53	0.44
1:B:1:MET:HE2	1:B:21:ASP:O	2.17	0.44
1:B:188:TYR:CE2	1:B:190:PRO:HB3	2.52	0.44
1:B:597:ILE:HD11	1:B:663:ILE:HG23	1.99	0.44
1:B:739:LYS:O	1:B:742:GLN:N	2.50	0.44
1:B:773:GLN:CD	1:B:773:GLN:N	2.76	0.44
1:C:19:TYR:N	1:C:19:TYR:CD1	2.86	0.44
1:D:1:MET:O	1:D:2:LYS:O	2.35	0.44
1:D:443:ILE:HD13	1:D:595:GLN:OE1	2.18	0.44
1:D:575:PHE:O	1:D:577:TYR:N	2.51	0.44
1:D:578:TYR:OH	1:D:580:LEU:HD23	2.18	0.44
1:D:625:ILE:HG23	1:D:683:MET:HE1	2.00	0.44
1:A:815:ILE:HG22	1:A:857:LEU:HD11	1.99	0.44
1:B:115:ILE:CG1	1:B:116:GLU:H	2.24	0.44
1:B:481:GLN:NE2	1:B:559:ARG:NE	2.56	0.44
1:B:506:PRO:CB	1:B:535:ALA:HB2	2.48	0.44
1:B:555:ALA:O	1:B:559:ARG:HG2	2.18	0.44
1:B:729:GLY:O	1:B:734:LYS:HE2	2.17	0.44
1:C:678:GLN:HG2	1:C:680:LEU:HG	1.99	0.44
1:D:830:VAL:CG2	1:D:831:TYR:N	2.81	0.44
3:F:105:DC:H2'	3:F:106:DT:H72	2.00	0.44
3:H:104:DG:C1'	3:H:105:DC:H5''	2.47	0.44
1:A:497:GLU:C	1:A:499:ILE:N	2.72	0.44
1:B:425:ILE:HG23	1:B:463:TYR:CE2	2.53	0.44
1:C:148:VAL:HG11	1:C:325:ILE:HD11	1.99	0.44
1:C:274:ILE:HG23	1:C:275:ASP:N	2.32	0.44
1:D:137:THR:CG2	1:D:328:VAL:HG21	2.47	0.44
1:D:274:ILE:CG1	1:D:278:LYS:HE3	2.47	0.44
1:D:395:PHE:CE2	1:D:397:LYS:HB2	2.53	0.44
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.53	0.44
1:D:495:ASN:OD1	1:D:521:ASP:HA	2.18	0.44
1:A:362:ILE:HD11	1:A:569:ALA:HA	1.99	0.43
1:A:702:TRP:CD1	1:A:708:TYR:HB3	2.53	0.43
1:A:725:LEU:HD22	1:A:753:LEU:HD12	1.99	0.43
1:A:784:SER:HB3	1:A:829:LYS:NZ	2.33	0.43
1:B:115:ILE:CG1	1:B:116:GLU:N	2.77	0.43
1:B:180:SER:O	1:B:183:ILE:HG22	2.19	0.43
1:B:434:PHE:HD1	1:B:462:MET:HG3	1.83	0.43
1:B:582:ASN:O	1:B:586:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:ILE:HD11	1:B:866:MET:HE1	1.99	0.43
1:C:97:TYR:O	1:C:99:TYR:N	2.47	0.43
1:C:523:SER:O	1:C:527:LYS:HG3	2.18	0.43
1:C:637:GLY:O	1:C:640:LYS:HB2	2.18	0.43
1:D:364:THR:HG22	1:D:365:TRP:N	2.33	0.43
1:D:421:ARG:NH1	1:D:479:PHE:CE2	2.84	0.43
3:J:105:DC:H2"	3:J:106:DT:C6	2.53	0.43
1:A:144:ASP:OD2	1:A:185:LYS:HE2	2.18	0.43
1:B:3:GLU:HG3	1:B:21:ASP:HA	1.99	0.43
1:B:197:LEU:C	1:B:197:LEU:CD2	2.91	0.43
1:C:187:ILE:O	1:C:187:ILE:HG22	2.18	0.43
1:C:297:GLU:OE1	1:C:338:ARG:NH1	2.51	0.43
1:D:140:ASP:OD1	1:D:141:SER:N	2.51	0.43
1:D:248:THR:HG21	1:D:265:LEU:HD23	1.99	0.43
1:D:285:GLN:C	1:D:287:SER:H	2.25	0.43
1:D:751:ARG:O	1:D:752:MET:C	2.62	0.43
1:A:1:MET:HE1	1:A:107:LYS:CE	2.48	0.43
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.98	0.43
1:A:707:ARG:HA	1:A:728:MET:O	2.18	0.43
1:B:301:GLY:O	1:B:302:LYS:HB2	2.18	0.43
1:D:23:ASN:HB2	1:D:24:GLY:H	1.57	0.43
1:D:118:THR:HG21	1:D:313:ARG:HB3	2.00	0.43
1:D:143:ASP:C	1:D:145:ARG:N	2.72	0.43
1:D:340:PHE:O	1:D:342:ASN:N	2.51	0.43
1:D:437:ALA:HB3	1:D:442:TYR:CE2	2.53	0.43
1:D:465:LYS:HZ2	1:D:675:ASN:CG	2.26	0.43
1:D:725:LEU:HD11	1:D:750:ARG:CB	2.48	0.43
1:A:89:LYS:HB2	1:A:89:LYS:NZ	2.33	0.43
1:A:429:THR:HG21	1:A:469:GLY:CA	2.47	0.43
1:A:596:TRP:CD1	1:A:596:TRP:C	2.96	0.43
1:B:162:TRP:CH2	1:B:186:ILE:HG21	2.54	0.43
1:B:308:PRO:C	1:B:310:SER:N	2.73	0.43
1:B:856:ASP:HA	1:B:859:LYS:HB2	2.00	0.43
1:C:20:ILE:CG2	1:C:24:GLY:HA2	2.49	0.43
1:C:510:VAL:O	1:C:510:VAL:HG12	2.18	0.43
1:C:514:LEU:HB2	1:C:541:MET:HE3	2.00	0.43
1:C:760:LEU:C	1:C:760:LEU:CD2	2.91	0.43
1:D:151:LEU:HA	1:D:191:PHE:O	2.19	0.43
1:A:75:MET:HE3	1:A:80:LEU:O	2.18	0.43
1:A:607:GLU:C	1:A:609:CYS:H	2.26	0.43
1:A:776:TYR:CG	1:A:863:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:PHE:CE1	1:A:813:ARG:HD2	2.53	0.43
1:B:191:PHE:CD1	1:B:197:LEU:HG	2.54	0.43
1:B:413:THR:O	1:B:414:SER:C	2.61	0.43
1:C:130:LYS:O	1:C:131:HIS:C	2.59	0.43
1:C:643:ASP:HB2	4:C:1005:HOH:O	2.17	0.43
1:D:270:VAL:O	1:D:271:LEU:HG	2.17	0.43
1:D:319:ARG:O	1:D:319:ARG:HD3	2.17	0.43
1:D:750:ARG:NH2	1:D:751:ARG:HG2	2.33	0.43
1:D:811:TYR:C	1:D:813:ARG:N	2.74	0.43
3:J:101:DG:C2'	3:J:102:DC:C6	3.01	0.43
1:B:528:GLU:C	1:B:530:ILE:N	2.77	0.43
1:B:898:PHE:C	1:B:900:MET:N	2.76	0.43
1:C:180:SER:O	1:C:182:ILE:N	2.51	0.43
1:C:398:GLU:OE1	1:C:705:LYS:HE3	2.18	0.43
1:C:458:PRO:HG2	1:C:592:MET:SD	2.58	0.43
1:C:512:GLU:HB3	1:C:513:PRO:CD	2.48	0.43
1:C:672:GLU:C	1:C:675:ASN:H	2.26	0.43
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.53	0.43
1:D:207:GLN:C	1:D:208:LYS:HG3	2.43	0.43
1:D:486:LYS:O	1:D:490:LEU:HG	2.19	0.43
1:D:550:VAL:CA	1:D:553:MET:HB3	2.45	0.43
1:D:859:LYS:O	1:D:863:LEU:HD22	2.19	0.43
1:A:277:TYR:C	1:A:279:LYS:N	2.77	0.43
1:A:373:LEU:HD12	1:A:380:ILE:HG22	2.00	0.43
1:A:458:PRO:HG3	1:A:592:MET:SD	2.58	0.43
1:A:482:ARG:HG2	1:A:482:ARG:HH11	1.84	0.43
1:B:6:LEU:HG	1:B:19:TYR:HA	1.99	0.43
1:C:411:ASP:CG	1:C:624:SER:HB3	2.44	0.43
1:C:811:TYR:HA	1:C:846:ILE:HD11	2.01	0.43
2:I:16:DG:C2'	2:I:17:DC:H5''	2.48	0.43
1:A:426:SER:OG	1:A:427:PRO:HD2	2.18	0.43
1:A:518:TYR:H	1:A:518:TYR:HD1	1.62	0.43
1:B:636:VAL:O	1:B:637:GLY:O	2.37	0.43
1:B:810:THR:CG2	1:B:841:PHE:HB3	2.49	0.43
1:B:861:ASP:C	1:B:863:LEU:H	2.26	0.43
1:C:138:HIS:C	1:C:138:HIS:CD2	2.97	0.43
1:C:181:GLU:H	1:C:181:GLU:CD	2.26	0.43
1:D:405:LYS:O	1:D:699:GLY:HA3	2.18	0.43
1:D:811:TYR:HB2	1:D:846:ILE:HG13	2.01	0.43
1:A:304:LYS:HB2	1:A:304:LYS:HE3	1.69	0.43
1:A:385:SER:HB2	4:A:959:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HD2	1:A:556:GLN:HG2	2.01	0.43
1:B:117:VAL:HB	1:B:124:PRO:HG3	2.01	0.43
1:B:513:PRO:CA	1:B:541:MET:HE1	2.49	0.43
1:B:771:PHE:HD1	1:B:774:LEU:CD1	2.30	0.43
1:B:897:LEU:H	1:B:897:LEU:CD2	2.22	0.43
1:C:136:ILE:O	1:C:148:VAL:HA	2.19	0.43
1:C:503:LEU:HD21	1:C:538:LEU:HB2	2.00	0.43
1:D:38:PHE:CE2	1:D:59:ARG:HG2	2.54	0.43
1:D:830:VAL:HG22	1:D:831:TYR:O	2.19	0.43
2:E:16:DG:C2'	2:E:17:DC:H5''	2.49	0.43
1:A:121:ASP:OD1	1:A:121:ASP:N	2.52	0.43
1:A:787:ASN:HB3	1:A:790:LYS:HE2	2.01	0.43
1:A:795:GLY:O	1:A:813:ARG:CD	2.67	0.43
1:A:873:GLU:HA	1:A:877:ILE:HB	2.00	0.43
1:B:45:GLN:O	1:B:47:THR:HG23	2.18	0.43
1:B:153:ASN:HB3	1:B:158:ASN:CG	2.44	0.43
1:B:159:VAL:HB	1:B:317:HIS:CG	2.54	0.43
1:C:81:GLU:CG	1:C:384:ARG:HH22	2.32	0.43
1:D:4:PHE:CZ	1:D:20:ILE:HD13	2.53	0.43
1:D:83:LEU:HD22	1:D:381:PRO:HA	2.00	0.43
1:D:491:ALA:HA	1:D:521:ASP:OD1	2.19	0.43
1:D:497:GLU:O	1:D:497:GLU:HG3	2.19	0.43
3:H:109:DC:H6	3:H:109:DC:H2'	1.72	0.43
2:I:6:DA:H2''	2:I:7:DA:C5'	2.47	0.43
1:B:738:PRO:HB2	1:B:778:SER:O	2.19	0.42
1:B:751:ARG:HA	1:B:755:GLU:HB2	2.01	0.42
1:C:135:ALA:O	1:C:136:ILE:CG1	2.66	0.42
1:C:540:GLU:O	1:C:544:ARG:HD3	2.18	0.42
1:C:725:LEU:HD11	1:C:750:ARG:HB2	2.01	0.42
1:D:206:GLN:NE2	1:D:241:ARG:HD2	2.34	0.42
1:D:294:SER:OG	1:D:330:ARG:HG2	2.19	0.42
1:D:586:ILE:HG22	1:D:587:THR:N	2.34	0.42
1:D:770:GLU:O	1:D:774:LEU:HG	2.18	0.42
1:A:752:MET:HG3	1:A:760:LEU:HD22	2.01	0.42
1:B:202:LEU:O	1:B:205:TRP:HB3	2.19	0.42
1:B:278:LYS:HG2	1:B:288:TYR:CE1	2.53	0.42
1:B:405:LYS:HG2	1:B:406:TYR:CD1	2.54	0.42
1:C:164:ILE:O	1:C:164:ILE:HG12	2.18	0.42
1:C:195:LYS:O	1:C:234:PHE:HZ	2.01	0.42
1:C:298:LEU:O	1:C:299:ASN:CB	2.67	0.42
1:D:262:ILE:O	1:D:262:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:LEU:HD11	1:D:333:GLN:CB	2.49	0.42
1:D:659:MET:O	1:D:660:GLU:C	2.61	0.42
3:L:110:DA:C2'	3:L:111:DT:H5''	2.49	0.42
1:A:240:LYS:C	1:A:242:LEU:N	2.76	0.42
1:A:808:ILE:O	1:A:811:TYR:HB3	2.18	0.42
1:B:45:GLN:NE2	1:B:58:THR:OG1	2.53	0.42
1:B:126:PRO:HB3	1:B:224:PRO:HB2	2.01	0.42
1:B:198:LEU:O	1:B:201:TYR:N	2.52	0.42
1:B:745:LEU:O	1:B:749:ILE:HG13	2.19	0.42
1:B:771:PHE:CD1	1:B:774:LEU:HD12	2.51	0.42
1:B:772:ARG:NH1	1:B:868:TYR:CB	2.82	0.42
1:C:362:ILE:CD1	1:C:575:PHE:HB2	2.50	0.42
1:C:416:TYR:HB2	1:C:417:PRO:HD3	2.01	0.42
1:C:542:LEU:O	1:C:546:GLN:HG3	2.19	0.42
1:C:745:LEU:HD23	1:C:745:LEU:HA	1.85	0.42
1:D:425:ILE:O	1:D:426:SER:HB2	2.19	0.42
1:D:496:GLY:HA2	1:D:499:ILE:HD12	2.01	0.42
1:D:747:GLU:HA	1:D:747:GLU:OE2	2.19	0.42
1:D:843:ASP:HB3	1:D:844:LYS:H	1.56	0.42
3:L:110:DA:C1'	3:L:111:DT:H5''	2.47	0.42
1:A:581:ARG:NH1	1:A:581:ARG:HB2	2.34	0.42
1:A:738:PRO:HB3	1:A:780:ALA:O	2.19	0.42
1:B:841:PHE:CZ	1:B:846:ILE:HD12	2.54	0.42
1:C:85:MET:HA	1:C:380:ILE:HD11	2.02	0.42
1:C:148:VAL:C	1:C:149:PHE:CD1	2.97	0.42
1:C:458:PRO:CG	1:C:592:MET:SD	3.07	0.42
1:C:516:VAL:HG12	1:C:526:ILE:HD13	2.01	0.42
1:A:439:LEU:O	1:A:443:ILE:HG13	2.19	0.42
1:A:523:SER:O	1:A:527:LYS:CB	2.68	0.42
1:B:218:VAL:HG23	1:B:219:GLU:N	2.33	0.42
1:B:299:ASN:N	1:B:299:ASN:ND2	2.66	0.42
1:B:494:ARG:HG3	1:B:495:ASN:ND2	2.35	0.42
1:D:115:ILE:HA	1:D:135:ALA:O	2.20	0.42
1:D:405:LYS:O	1:D:690:GLY:HA2	2.19	0.42
1:D:459:ASN:C	1:D:459:ASN:HD22	2.27	0.42
1:D:481:GLN:CB	1:D:559:ARG:NE	2.69	0.42
1:D:632:ILE:C	1:D:634:ASP:H	2.27	0.42
1:D:805:ILE:HD13	1:D:808:ILE:HD12	2.01	0.42
3:H:109:DC:H1'	3:H:110:DA:H5'	2.01	0.42
1:A:83:LEU:N	1:A:83:LEU:HD12	2.35	0.42
1:A:861:ASP:O	1:A:864:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:OD2	1:B:318:GLN:HG3	2.19	0.42
1:B:671:CYS:SG	1:B:676:ASN:HB2	2.59	0.42
1:B:846:ILE:HG23	1:B:846:ILE:O	2.19	0.42
1:C:500:LYS:HE2	1:C:542:LEU:HD21	2.01	0.42
1:D:25:ARG:NH1	1:D:25:ARG:CG	2.81	0.42
1:D:151:LEU:HG	1:D:192:ASP:O	2.18	0.42
1:D:403:ARG:NH2	1:D:698:ILE:HG22	2.33	0.42
1:D:503:LEU:HG	1:D:538:LEU:HB3	2.01	0.42
1:D:761:GLN:HE22	1:D:893:LYS:HA	1.82	0.42
1:D:873:GLU:HA	1:D:877:ILE:HB	2.02	0.42
1:A:702:TRP:CZ3	1:A:710:LEU:HD21	2.54	0.42
1:A:725:LEU:HD11	1:A:750:ARG:HB2	2.02	0.42
1:A:862:VAL:C	1:A:864:HIS:N	2.74	0.42
1:B:4:PHE:O	1:B:19:TYR:HB2	2.19	0.42
1:B:202:LEU:CD1	1:B:242:LEU:HD13	2.50	0.42
1:B:228:ASN:O	1:B:231:LYS:HG2	2.20	0.42
1:B:236:GLU:O	1:B:237:SER:C	2.62	0.42
1:B:475:ILE:HD13	1:B:566:LEU:HG	2.01	0.42
1:B:658:ARG:CD	1:D:897:LEU:HD22	2.46	0.42
1:C:9:GLU:OE1	1:C:266:PHE:HA	2.19	0.42
1:C:203:ASN:N	1:C:203:ASN:ND2	2.68	0.42
1:C:243:SER:C	1:C:245:HIS:H	2.27	0.42
1:C:266:PHE:N	1:C:266:PHE:CD1	2.87	0.42
1:D:291:ASP:O	1:D:292:TYR:C	2.62	0.42
1:D:294:SER:C	1:D:296:PHE:H	2.28	0.42
1:D:848:TRP:HB2	4:D:918:HOH:O	2.19	0.42
2:E:6:DA:C1'	2:E:7:DA:H5''	2.45	0.42
2:K:16:DG:H5'	4:K:30:HOH:O	2.20	0.42
1:A:2:LYS:N	1:A:2:LYS:CD	2.68	0.42
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.55	0.42
1:A:559:ARG:HA	1:A:562:LEU:HD23	2.01	0.42
1:B:48:LYS:O	1:B:377:ASN:HB3	2.20	0.42
1:B:315:SER:OG	1:B:316:ASN:N	2.52	0.42
1:B:732:THR:HG22	1:B:745:LEU:HB3	2.02	0.42
1:C:728:MET:HE2	3:J:114:DA:OP2	2.19	0.42
1:D:219:GLU:HB3	1:D:272:ASP:OD2	2.19	0.42
1:D:247:LYS:O	1:D:266:PHE:HB2	2.20	0.42
1:D:391:TYR:HB2	1:D:392:PRO:CD	2.34	0.42
1:D:743:LYS:HE3	1:D:743:LYS:HB2	1.90	0.42
1:D:760:LEU:C	1:D:760:LEU:CD2	2.93	0.42
2:E:10:DA:C2'	2:E:11:DC:C5'	2.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:HB2	1:A:591:GLN:CG	2.34	0.42
1:B:3:GLU:HG3	1:B:20:ILE:O	2.20	0.42
1:B:118:THR:HG23	1:B:118:THR:O	2.19	0.42
1:B:365:TRP:CD2	1:B:566:LEU:HD23	2.55	0.42
1:B:709:ALA:HA	1:B:726:LYS:O	2.20	0.42
1:B:853:GLU:O	1:B:854:ILE:C	2.63	0.42
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.55	0.42
1:C:326:ILE:HD12	1:C:326:ILE:C	2.43	0.42
1:C:572:ASN:O	1:C:578:TYR:HB2	2.20	0.42
1:D:7:THR:HG22	1:D:18:ARG:CB	2.48	0.42
1:D:20:ILE:HD12	1:D:107:LYS:CB	2.50	0.42
1:D:597:ILE:HA	1:D:597:ILE:HD12	1.82	0.42
1:D:599:ARG:HG2	1:D:599:ARG:NH1	2.34	0.42
1:D:614:GLU:HG2	1:D:631:LYS:HE3	2.02	0.42
1:D:628:SER:C	1:D:630:ASP:H	2.27	0.42
3:F:113:DC:H2''	3:F:114:DA:OP2	2.18	0.42
3:L:110:DA:H2''	3:L:111:DT:H5'	2.02	0.42
1:B:200:GLU:O	1:B:201:TYR:C	2.63	0.42
1:B:372:SER:OG	1:B:474:GLU:OE1	2.31	0.42
1:B:415:LEU:HD11	1:B:681:MET:HE1	2.02	0.42
1:B:426:SER:HB2	1:B:472:PRO:HD2	2.02	0.42
1:B:708:TYR:CE1	1:B:728:MET:HB2	2.55	0.42
1:C:3:GLU:HG2	1:C:21:ASP:CA	2.46	0.42
1:C:178:VAL:O	1:C:179:PRO:O	2.38	0.42
1:D:323:TYR:CE1	1:D:326:ILE:HD12	2.54	0.42
1:D:376:GLN:O	1:D:377:ASN:HB2	2.18	0.42
1:D:484:GLU:O	1:D:486:LYS:N	2.53	0.42
1:D:495:ASN:HD21	1:D:521:ASP:HA	1.85	0.42
1:D:508:LEU:H	1:D:508:LEU:CD2	2.28	0.42
1:D:708:TYR:CE1	1:D:728:MET:HB3	2.55	0.42
2:E:16:DG:H2''	2:E:17:DC:H5''	2.01	0.42
1:A:709:ALA:HA	1:A:726:LYS:O	2.20	0.41
1:B:480:ASN:O	1:B:483:LYS:HB2	2.20	0.41
1:B:644:THR:O	1:B:645:ASN:C	2.63	0.41
1:B:662:ALA:HA	1:B:665:ARG:NH2	2.35	0.41
1:B:877:ILE:O	1:B:878:LYS:C	2.62	0.41
1:C:199:MET:HG2	1:C:234:PHE:CE2	2.55	0.41
1:C:303:LEU:HD21	1:C:319:ARG:CG	2.49	0.41
1:C:377:ASN:HD22	1:C:377:ASN:HA	1.68	0.41
1:C:592:MET:HE3	1:C:670:MET:SD	2.60	0.41
1:D:7:THR:CG2	1:D:18:ARG:HE	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:HG2	1:D:319:ARG:NH1	2.33	0.41
1:D:351:ALA:O	1:D:352:LYS:HB2	2.19	0.41
1:D:729:GLY:N	3:L:113:DC:OP1	2.44	0.41
3:F:103:DG:C2'	3:F:104:DG:H5'	2.49	0.41
3:L:106:DT:H2''	3:L:107:DG:OP2	2.20	0.41
1:A:529:LYS:O	1:A:533:LEU:HD11	2.20	0.41
1:A:839:ASN:HA	1:A:840:PRO:HD3	1.77	0.41
1:B:231:LYS:HB2	1:B:231:LYS:HE3	1.83	0.41
1:B:592:MET:HE1	1:B:674:MET:HG3	2.02	0.41
1:B:737:THR:HG22	1:B:738:PRO:HD2	2.02	0.41
1:C:660:GLU:CB	1:C:661:PRO:CD	2.97	0.41
1:D:17:GLU:CG	1:D:18:ARG:N	2.82	0.41
1:D:273:TYR:HD1	1:D:273:TYR:O	2.03	0.41
1:D:423:VAL:O	1:D:424:ASN:CB	2.68	0.41
1:D:488:TYR:HE2	1:D:519:ARG:HD2	1.85	0.41
1:A:277:TYR:C	1:A:279:LYS:H	2.27	0.41
1:B:186:ILE:HG22	1:B:187:ILE:H	1.85	0.41
1:B:353:ILE:O	1:B:354:GLN:C	2.61	0.41
1:B:598:GLU:HG3	1:B:617:VAL:HG11	2.02	0.41
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.55	0.41
1:C:457:SER:O	1:C:459:ASN:N	2.53	0.41
1:D:19:TYR:O	1:D:27:ARG:N	2.53	0.41
1:D:144:ASP:O	1:D:145:ARG:NE	2.53	0.41
1:D:217:ASN:N	1:D:272:ASP:OD1	2.53	0.41
1:D:283:THR:HG21	1:D:285:GLN:HE22	1.83	0.41
1:D:800:LYS:H	2:K:13:DG:C5'	2.33	0.41
1:D:830:VAL:CG2	1:D:847:ALA:HB1	2.51	0.41
1:C:162:TRP:CZ3	1:C:164:ILE:HB	2.55	0.41
1:C:167:ALA:O	1:C:176:ASP:O	2.38	0.41
1:C:189:MET:O	1:C:191:PHE:HE1	2.04	0.41
1:C:496:GLY:C	1:C:498:ILE:H	2.28	0.41
1:D:191:PHE:HD2	1:D:197:LEU:HA	1.83	0.41
1:D:285:GLN:HB3	1:D:292:TYR:HE2	1.86	0.41
1:D:355:ILE:C	1:D:357:SER:H	2.28	0.41
1:D:410:PHE:CD2	1:D:685:ARG:HA	2.56	0.41
1:D:449:ARG:HA	1:D:450:PRO:HD2	1.90	0.41
1:D:458:PRO:C	1:D:460:GLY:H	2.28	0.41
1:D:479:PHE:CD1	1:D:563:ILE:HD13	2.56	0.41
1:D:579:ASP:O	1:D:582:ASN:HB2	2.21	0.41
1:D:619:TYR:CD1	1:D:619:TYR:C	2.98	0.41
1:D:625:ILE:CG2	1:D:683:MET:HE1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DA:H2''	4:E:19:HOH:O	2.19	0.41
1:A:219:GLU:O	1:A:219:GLU:HG2	2.21	0.41
1:A:303:LEU:HD12	1:A:304:LYS:H	1.86	0.41
1:A:602:ASN:ND2	1:A:616:PHE:N	2.68	0.41
1:A:806:ARG:HD2	1:A:844:LYS:NZ	2.35	0.41
1:B:363:LYS:HD3	1:B:363:LYS:HA	1.84	0.41
1:B:395:PHE:HB2	1:B:591:GLN:CG	2.34	0.41
1:B:797:PRO:HB3	1:B:809:LEU:HD12	2.01	0.41
1:C:150:ASP:HB2	1:C:188:TYR:HE1	1.86	0.41
1:C:512:GLU:CB	1:C:513:PRO:HD2	2.48	0.41
1:C:514:LEU:CD1	1:C:530:ILE:HG12	2.51	0.41
1:D:110:VAL:HG11	1:D:341:ILE:HG21	2.03	0.41
1:D:243:SER:O	1:D:245:HIS:N	2.52	0.41
1:D:482:ARG:HB2	1:D:559:ARG:CB	2.36	0.41
1:D:543:PHE:HD1	1:D:546:GLN:HE22	1.67	0.41
1:D:556:GLN:C	1:D:556:GLN:CD	2.89	0.41
1:D:582:ASN:O	1:D:585:ALA:N	2.54	0.41
1:D:705:LYS:C	1:D:707:ARG:N	2.78	0.41
1:A:154:SER:O	1:A:156:TYR:N	2.53	0.41
1:A:351:ALA:O	1:A:352:LYS:HB2	2.19	0.41
1:B:221:PHE:HE2	1:B:225:TYR:HD1	1.67	0.41
1:B:351:ALA:O	1:B:352:LYS:HB2	2.20	0.41
1:B:678:GLN:O	1:B:680:LEU:HG	2.20	0.41
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.55	0.41
1:B:810:THR:HB	1:B:845:CYS:O	2.20	0.41
1:C:433:THR:O	1:C:462:MET:HE2	2.21	0.41
1:C:591:GLN:HE21	1:C:591:GLN:HB2	1.66	0.41
1:D:8:VAL:C	1:D:9:GLU:OE2	2.63	0.41
1:D:65:MET:HB3	1:D:88:PHE:CE2	2.55	0.41
1:D:98:ASN:O	1:D:99:TYR:HB3	2.20	0.41
1:D:449:ARG:NH2	1:D:675:ASN:HB2	2.18	0.41
1:A:526:ILE:HG22	1:A:530:ILE:CD1	2.45	0.41
1:B:302:LYS:HG2	1:B:303:LEU:N	2.36	0.41
1:B:343:LEU:HG	1:B:558:ASN:HD21	1.86	0.41
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.56	0.41
1:D:129:ALA:HA	1:D:225:TYR:HE1	1.84	0.41
1:D:370:PHE:CD2	1:D:370:PHE:C	2.97	0.41
1:D:415:LEU:O	1:D:419:ILE:HG13	2.21	0.41
1:D:421:ARG:HH11	1:D:421:ARG:HG3	1.86	0.41
1:D:544:ARG:HH11	1:D:544:ARG:HG3	1.85	0.41
1:A:395:PHE:CB	1:A:591:GLN:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ALA:O	1:A:630:ASP:C	2.63	0.41
1:B:198:LEU:HD13	1:B:230:ILE:HG12	2.03	0.41
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.89	0.41
1:C:80:LEU:HD22	1:C:80:LEU:N	2.35	0.41
1:C:362:ILE:HD13	1:C:362:ILE:HA	1.90	0.41
1:D:433:THR:N	1:D:462:MET:HE2	2.36	0.41
1:D:499:ILE:HB	1:D:542:LEU:HD13	2.03	0.41
3:F:111:DT:C1'	3:F:112:DT:H5''	2.50	0.41
2:G:13:DG:N2	3:H:105:DC:N3	2.60	0.41
1:A:37:LEU:HD11	1:A:72:ILE:HD11	2.03	0.41
1:A:517:ASP:C	1:A:519:ARG:H	2.29	0.41
1:A:655:ALA:HA	1:A:659:MET:HB2	2.03	0.41
1:B:365:TRP:CE2	1:B:566:LEU:HD23	2.55	0.41
1:B:699:GLY:C	1:B:753:LEU:HD22	2.46	0.41
1:B:707:ARG:NH1	1:B:729:GLY:O	2.54	0.41
1:B:813:ARG:C	1:B:815:ILE:H	2.28	0.41
1:B:846:ILE:HD11	1:B:858:ILE:CD1	2.25	0.41
1:B:900:MET:HE1	1:D:640:LYS:CE	2.50	0.41
1:C:151:LEU:CD2	1:C:152:LEU:N	2.84	0.41
1:C:274:ILE:CG2	1:C:275:ASP:N	2.83	0.41
1:D:81:GLU:HG2	1:D:83:LEU:CD2	2.51	0.41
1:D:136:ILE:HB	1:D:149:PHE:HB2	2.03	0.41
1:D:241:ARG:HD3	1:D:241:ARG:HA	1.95	0.41
1:D:380:ILE:HA	1:D:381:PRO:HD3	1.84	0.41
1:D:403:ARG:H	1:D:403:ARG:HG2	1.71	0.41
1:D:525:GLU:C	1:D:529:LYS:HE2	2.46	0.41
1:D:586:ILE:O	1:D:589:PHE:N	2.54	0.41
1:D:633:ILE:O	1:D:633:ILE:CG2	2.68	0.41
2:I:7:DA:C8	2:I:8:DT:H72	2.56	0.41
1:A:38:PHE:CE2	1:A:59:ARG:HB2	2.56	0.41
1:A:48:LYS:HG2	4:A:957:HOH:O	2.19	0.41
1:A:362:ILE:HD12	1:A:569:ALA:CA	2.48	0.41
1:A:423:VAL:O	1:A:424:ASN:HB3	2.21	0.41
1:A:661:PRO:O	1:A:665:ARG:HB2	2.21	0.41
1:B:496:GLY:O	1:B:542:LEU:HD13	2.21	0.41
1:B:606:ASN:ND2	1:B:613:GLY:H	2.19	0.41
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.56	0.41
1:C:2:LYS:HE2	1:C:102:LYS:CB	2.51	0.41
1:D:102:LYS:HB2	1:D:102:LYS:NZ	2.36	0.41
1:D:116:GLU:CB	1:D:320:TYR:OH	2.69	0.41
1:D:271:LEU:HD22	1:D:276:LEU:CD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:O	1:D:343:LEU:C	2.64	0.41
1:D:362:ILE:HG22	1:D:575:PHE:CD1	2.52	0.41
1:D:804:HIS:C	1:D:806:ARG:N	2.78	0.41
2:G:15:DC:H2''	2:G:16:DG:H5'	2.01	0.41
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.56	0.40
1:A:501:GLU:C	1:A:503:LEU:H	2.29	0.40
1:B:114:ASP:HB3	1:B:324:ASN:ND2	2.36	0.40
1:B:240:LYS:C	1:B:242:LEU:N	2.77	0.40
1:B:329:TYR:CE2	1:B:333:GLN:NE2	2.89	0.40
1:B:330:ARG:HA	1:B:333:GLN:HB2	2.03	0.40
1:B:690:GLY:O	1:B:711:ASN:HB3	2.21	0.40
1:B:781:SER:HB2	1:B:832:VAL:HB	2.03	0.40
1:C:44:SER:C	1:C:46:ALA:H	2.29	0.40
1:D:189:MET:O	1:D:191:PHE:HD1	2.05	0.40
1:D:825:VAL:CG1	1:D:826:GLU:H	2.32	0.40
1:A:402:ASN:CG	1:A:403:ARG:N	2.79	0.40
1:B:1:MET:CE	1:B:24:GLY:HA2	2.49	0.40
1:B:125:GLU:C	1:B:127:SER:N	2.79	0.40
1:B:154:SER:C	1:B:156:TYR:H	2.28	0.40
1:B:491:ALA:HB3	1:B:519:ARG:O	2.21	0.40
1:B:494:ARG:CG	1:B:495:ASN:ND2	2.84	0.40
1:C:6:LEU:C	1:C:7:THR:HG23	2.45	0.40
1:C:353:ILE:HD12	1:C:357:SER:HB2	2.03	0.40
1:D:118:THR:O	1:D:313:ARG:NH2	2.53	0.40
1:D:183:ILE:HG23	1:D:184:ASP:N	2.36	0.40
1:D:198:LEU:CD2	1:D:230:ILE:HG12	2.49	0.40
1:D:223:ILE:CB	1:D:224:PRO:HD3	2.43	0.40
1:D:698:ILE:HG13	1:D:753:LEU:HD23	2.02	0.40
1:A:38:PHE:HE2	1:A:59:ARG:HB2	1.86	0.40
1:A:152:LEU:HD11	1:A:190:PRO:HB2	2.02	0.40
1:A:530:ILE:C	1:A:532:LYS:H	2.30	0.40
1:A:566:LEU:CD1	1:A:570:LEU:HD22	2.52	0.40
1:A:745:LEU:HA	1:A:745:LEU:HD12	1.77	0.40
1:B:728:MET:C	1:B:730:LEU:H	2.30	0.40
1:C:40:HIS:HE1	1:C:51:ASP:OD2	2.04	0.40
1:C:139:TYR:CD1	1:C:139:TYR:C	2.99	0.40
1:C:529:LYS:O	1:C:529:LYS:CG	2.69	0.40
1:C:605:LEU:HD13	1:C:616:PHE:CD2	2.56	0.40
1:D:516:VAL:CG1	1:D:526:ILE:HD13	2.52	0.40
1:D:692:PRO:HG3	1:D:713:TRP:CZ2	2.56	0.40
1:D:791:TYR:HB2	1:D:805:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:LEU:HD22	1:D:863:LEU:H	1.86	0.40
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.57	0.40
1:A:386:HIS:HB2	1:A:573:VAL:HB	2.04	0.40
1:A:636:VAL:O	1:A:636:VAL:CG1	2.69	0.40
1:B:108:ILE:O	1:B:110:VAL:HG23	2.21	0.40
1:B:520:PHE:O	1:B:521:ASP:C	2.64	0.40
1:C:218:VAL:HA	1:C:222:ALA:HB3	2.04	0.40
1:C:227:TYR:CD2	1:C:228:ASN:ND2	2.88	0.40
1:C:423:VAL:HB	1:C:425:ILE:HG13	2.03	0.40
1:C:727:ILE:HD13	1:C:749:ILE:CD1	2.51	0.40
1:D:542:LEU:C	1:D:544:ARG:N	2.78	0.40
1:B:26:GLU:C	1:B:27:ARG:HG2	2.47	0.40
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.89	0.40
1:B:566:LEU:C	1:B:566:LEU:HD13	2.45	0.40
1:B:596:TRP:CD1	1:B:596:TRP:C	2.99	0.40
1:C:166:ILE:C	1:C:168:ALA:H	2.29	0.40
1:C:250:VAL:HG23	1:C:261:GLU:OE2	2.21	0.40
1:D:198:LEU:HD12	1:D:198:LEU:N	2.37	0.40
1:D:217:ASN:OD1	1:D:217:ASN:O	2.40	0.40
1:D:272:ASP:HB3	1:D:274:ILE:HG22	2.03	0.40
1:D:319:ARG:HD3	1:D:323:TYR:CD1	2.56	0.40
1:D:535:ALA:O	1:D:539:ASN:ND2	2.54	0.40
1:D:837:GLU:H	1:D:837:GLU:HG2	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	867/906 (96%)	781 (90%)	74 (8%)	12 (1%)	9	18
1	B	884/906 (98%)	756 (86%)	103 (12%)	25 (3%)	4	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	886/906 (98%)	769 (87%)	94 (11%)	23 (3%)	4	9
1	D	886/906 (98%)	681 (77%)	162 (18%)	43 (5%)	1	2
All	All	3523/3624 (97%)	2987 (85%)	433 (12%)	103 (3%)	3	8

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
1	A	534	SER
1	B	121	ASP
1	B	236	GLU
1	B	306	ASP
1	B	534	SER
1	B	637	GLY
1	B	802	PRO
1	C	315	SER
1	D	2	LYS
1	D	21	ASP
1	D	23	ASN
1	D	106	THR
1	D	305	TYR
1	D	344	SER
1	D	611	THR
1	D	630	ASP
1	B	115	ILE
1	B	179	PRO
1	B	199	MET
1	B	304	LYS
1	C	24	GLY
1	C	120	PRO
1	C	181	GLU
1	C	232	ASN
1	C	607	GLU
1	D	10	GLN
1	D	29	ARG
1	D	45	GLN
1	D	129	ALA
1	D	295	GLU
1	D	306	ASP
1	D	508	LEU
1	D	576	ARG

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Mol	Chain	Res	Type
1	D	631	LYS
1	D	656	ARG
1	D	843	ASP
1	A	99	TYR
1	A	843	ASP
1	B	272	ASP
1	B	537	SER
1	B	645	ASN
1	B	800	LYS
1	B	858	ILE
1	C	159	VAL
1	C	179	PRO
1	C	299	ASN
1	C	311	LYS
1	C	622	THR
1	D	24	GLY
1	D	169	LYS
1	D	291	ASP
1	D	405	LYS
1	D	450	PRO
1	D	521	ASP
1	D	622	THR
1	D	739	LYS
1	D	754	GLN
1	A	169	LYS
1	B	739	LYS
1	B	774	LEU
1	C	63	ALA
1	C	112	ASN
1	C	135	ALA
1	C	301	GLY
1	C	458	PRO
1	C	484	GLU
1	D	459	ASN
1	D	579	ASP
1	D	850	SER
1	D	897	LEU
1	A	284	ASN
1	A	498	ILE
1	B	523	SER
1	C	98	ASN
1	C	177	GLU

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	785/803 (98%)	749 (95%)	36 (5%)	24	48
1	B	774/803 (96%)	739 (96%)	35 (4%)	24	48
1	C	780/803 (97%)	743 (95%)	37 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	764/803 (95%)	726 (95%)	38 (5%)	22	44
All	All	3103/3212 (97%)	2957 (95%)	146 (5%)	23	47

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	22	SER
1	A	25	ARG
1	A	35	PRO
1	A	58	THR
1	A	89	LYS
1	A	100	GLU
1	A	101	ILE
1	A	128	GLN
1	A	134	ASP
1	A	154	SER
1	A	200	GLU
1	A	203	ASN
1	A	217	ASN
1	A	231	LYS
1	A	242	LEU
1	A	246	ARG
1	A	264	THR
1	A	352	LYS
1	A	358	VAL
1	A	362	ILE
1	A	379	VAL
1	A	474	GLU
1	A	479	PHE
1	A	562	LEU
1	A	570	LEU
1	A	581	ARG
1	A	718	THR
1	A	731	GLU
1	A	739	LYS
1	A	745	LEU
1	A	765	LYS
1	A	799	PRO
1	A	825	VAL
1	A	855	THR
1	A	893	LYS

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Mol	Chain	Res	Type
1	B	22	SER
1	B	27	ARG
1	B	28	THR
1	B	37	LEU
1	B	58	THR
1	B	61	LEU
1	B	113	PHE
1	B	117	VAL
1	B	123	PHE
1	B	133	ILE
1	B	136	ILE
1	B	179	PRO
1	B	199	MET
1	B	234	PHE
1	B	261	GLU
1	B	273	TYR
1	B	303	LEU
1	B	334	ILE
1	B	337	LYS
1	B	338	ARG
1	B	428	GLU
1	B	479	PHE
1	B	483	LYS
1	B	497	GLU
1	B	541	MET
1	B	562	LEU
1	B	580	LEU
1	B	635	LYS
1	B	722	GLU
1	B	731	GLU
1	B	755	GLU
1	B	760	LEU
1	B	773	GLN
1	B	878	LYS
1	B	897	LEU
1	C	15	ILE
1	C	19	TYR
1	C	27	ARG
1	C	28	THR
1	C	58	THR
1	C	90	LEU
1	C	105	HIS

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Mol	Chain	Res	Type
1	C	128	GLN
1	C	132	PRO
1	C	148	VAL
1	C	151	LEU
1	C	213	LEU
1	C	217	ASN
1	C	219	GLU
1	C	231	LYS
1	C	250	VAL
1	C	281	SER
1	C	283	THR
1	C	332	LEU
1	C	342	ASN
1	C	356	GLN
1	C	411	ASP
1	C	428	GLU
1	C	436	VAL
1	C	440	HIS
1	C	456	CYS
1	C	475	ILE
1	C	479	PHE
1	C	562	LEU
1	C	591	GLN
1	C	608	VAL
1	C	642	ARG
1	C	660	GLU
1	C	731	GLU
1	C	760	LEU
1	C	878	LYS
1	C	898	PHE
1	D	4	PHE
1	D	9	GLU
1	D	15	ILE
1	D	19	TYR
1	D	20	ILE
1	D	25	ARG
1	D	48	LYS
1	D	59	ARG
1	D	61	LEU
1	D	90	LEU
1	D	102	LYS
1	D	134	ASP

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Mol	Chain	Res	Type
1	D	145	ARG
1	D	146	PHE
1	D	199	MET
1	D	206	GLN
1	D	272	ASP
1	D	282	PHE
1	D	330	ARG
1	D	362	ILE
1	D	363	LYS
1	D	428	GLU
1	D	459	ASN
1	D	474	GLU
1	D	475	ILE
1	D	485	HIS
1	D	524	ASP
1	D	553	MET
1	D	557	ILE
1	D	580	LEU
1	D	618	LEU
1	D	633	ILE
1	D	646	HIS
1	D	649	ASP
1	D	686	GLU
1	D	755	GLU
1	D	828	GLU
1	D	844	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	40	HIS
1	A	45	GLN
1	A	173	GLN
1	A	206	GLN
1	A	217	ASN
1	A	284	ASN
1	A	356	GLN
1	A	371	ASN
1	A	377	ASN
1	A	422	GLN
1	A	481	GLN

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Mol	Chain	Res	Type
1	A	485	HIS
1	A	493	GLN
1	A	507	ASN
1	A	546	GLN
1	A	556	GLN
1	A	558	ASN
1	A	595	GLN
1	A	602	ASN
1	A	678	GLN
1	A	742	GLN
1	A	786	ASN
1	A	787	ASN
1	A	812	ASN
1	A	864	HIS
1	B	40	HIS
1	B	45	GLN
1	B	70	GLN
1	B	112	ASN
1	B	173	GLN
1	B	203	ASN
1	B	245	HIS
1	B	299	ASN
1	B	316	ASN
1	B	317	HIS
1	B	318	GLN
1	B	324	ASN
1	B	333	GLN
1	B	354	GLN
1	B	376	GLN
1	B	389	GLN
1	B	481	GLN
1	B	495	ASN
1	B	558	ASN
1	B	595	GLN
1	B	606	ASN
1	B	645	ASN
1	B	761	GLN
1	B	812	ASN
1	B	818	ASN
1	C	10	GLN
1	C	40	HIS
1	C	45	GLN

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Mol	Chain	Res	Type
1	C	173	GLN
1	C	203	ASN
1	C	207	GLN
1	C	217	ASN
1	C	228	ASN
1	C	232	ASN
1	C	284	ASN
1	C	318	GLN
1	C	324	ASN
1	C	339	GLN
1	C	354	GLN
1	C	356	GLN
1	C	377	ASN
1	C	386	HIS
1	C	424	ASN
1	C	481	GLN
1	C	495	ASN
1	C	507	ASN
1	C	539	ASN
1	C	546	GLN
1	C	556	GLN
1	C	558	ASN
1	C	591	GLN
1	C	645	ASN
1	C	733	GLN
1	C	773	GLN
1	C	818	ASN
1	D	40	HIS
1	D	45	GLN
1	D	64	ASN
1	D	131	HIS
1	D	138	HIS
1	D	206	GLN
1	D	207	GLN
1	D	285	GLN
1	D	316	ASN
1	D	324	ASN
1	D	354	GLN
1	D	376	GLN
1	D	389	GLN
1	D	402	ASN
1	D	422	GLN

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Mol	Chain	Res	Type
1	D	444	ASN
1	D	504	HIS
1	D	546	GLN
1	D	556	GLN
1	D	558	ASN
1	D	591	GLN
1	D	676	ASN
1	D	679	HIS
1	D	733	GLN
1	D	773	GLN
1	D	775	ASN
1	D	787	ASN
1	D	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CTG	I	4	3,2	18,23,24	0.99	2 (11%)	21,35,38	0.63	1 (4%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C5-C4	2.91	1.55	1.52
2	I	4	CTG	C1'-N1	2.11	1.48	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	CTG	N3-C2-N1	-2.31	114.36	116.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	894/906 (98%)	-0.26	9 (1%) 79 75	19, 41, 114, 141	1 (0%)
1	B	897/906 (99%)	0.43	100 (11%) 10 8	26, 61, 157, 177	13 (1%)
1	C	890/906 (98%)	-0.10	11 (1%) 76 71	19, 49, 103, 130	2 (0%)
1	D	890/906 (98%)	0.96	109 (12%) 8 6	60, 102, 147, 163	5 (0%)
2	E	14/18 (77%)	0.54	1 (7%) 22 16	69, 87, 126, 130	0
2	G	13/18 (72%)	1.20	1 (7%) 19 15	59, 143, 168, 169	0
2	I	16/18 (88%)	-0.47	0 100 100	33, 45, 113, 113	0
2	K	12/18 (66%)	0.50	0 100 100	41, 116, 144, 150	0
3	F	14/14 (100%)	0.64	1 (7%) 22 16	87, 103, 120, 132	0
3	H	13/14 (92%)	1.07	2 (15%) 5 4	137, 149, 163, 168	0
3	J	14/14 (100%)	-0.00	1 (7%) 22 16	35, 61, 89, 93	0
3	L	13/14 (92%)	0.78	0 100 100	119, 128, 134, 138	0
All	All	3680/3752 (98%)	0.27	235 (6%) 25 20	19, 63, 144, 177	21 (0%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	862	VAL	5.7
1	B	847	ALA	5.1
1	B	799	PRO	4.8
1	D	252	VAL	4.7
1	B	846	ILE	4.7
1	B	132	PRO	4.5
1	B	865	TRP	4.4
1	D	779	ILE	4.3
1	B	864	HIS	4.3
1	B	844	LYS	4.3
1	B	863	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	286	PRO	4.2
1	D	393	GLY	4.2
1	B	803	PHE	4.2
1	D	394	ALA	4.1
1	B	504	HIS	4.1
1	D	138	HIS	4.1
1	B	811	TYR	4.0
1	D	526	ILE	4.0
1	B	117	VAL	4.0
1	D	782	VAL	3.9
1	B	819	ILE	3.8
1	D	156	TYR	3.8
1	D	20	ILE	3.8
1	D	498	ILE	3.7
1	B	821	ALA	3.7
1	B	309	ILE	3.7
1	A	508	LEU	3.6
1	B	834	PRO	3.6
1	D	850	SER	3.6
1	B	802	PRO	3.6
1	B	123	PHE	3.6
1	B	133	ILE	3.5
1	D	170	LEU	3.5
1	B	782	VAL	3.4
1	B	798	GLY	3.4
1	B	809	LEU	3.4
1	D	117	VAL	3.4
1	D	113	PHE	3.3
1	B	800	LYS	3.3
2	G	6	DA	3.3
1	B	866	MET	3.3
1	D	171	GLN	3.3
1	B	825	VAL	3.2
1	D	848	TRP	3.2
1	B	785	ALA	3.2
1	D	202	LEU	3.2
1	D	178	VAL	3.2
1	B	868	TYR	3.1
1	C	168	ALA	3.1
1	B	156	TYR	3.1
1	B	776	TYR	3.1
3	F	114	DA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	498	ILE	3.1
1	D	831	TYR	3.0
1	B	861	ASP	3.0
1	B	801	CYS	3.0
1	D	213	LEU	3.0
1	B	845	CYS	3.0
1	C	508	LEU	3.0
1	D	303	LEU	3.0
1	A	510	VAL	3.0
1	D	173	GLN	3.0
1	B	118	THR	3.0
1	B	301	GLY	3.0
1	B	796	PHE	3.0
3	J	114	DA	3.0
1	B	795	GLY	2.9
1	D	265	LEU	2.9
1	D	508	LEU	2.9
1	D	395	PHE	2.9
1	D	800	LYS	2.9
1	B	779	ILE	2.9
1	D	525	GLU	2.9
1	D	832	VAL	2.9
1	B	833	LEU	2.9
1	D	812	ASN	2.9
1	C	510	VAL	2.9
1	D	514	LEU	2.9
1	D	784	SER	2.8
1	B	131	HIS	2.8
1	B	503	LEU	2.8
1	D	164	ILE	2.8
1	B	505	ASN	2.8
1	D	522	PHE	2.8
1	B	514	LEU	2.8
1	D	262	ILE	2.8
3	H	101	DG	2.8
1	D	535	ALA	2.7
1	B	780	ALA	2.7
1	D	298	LEU	2.7
1	D	264	THR	2.7
1	D	290	LEU	2.7
1	D	542	LEU	2.7
1	B	194	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	282	PHE	2.6
1	B	832	VAL	2.6
1	A	526	ILE	2.6
1	D	15	ILE	2.6
1	D	263	ILE	2.6
1	D	814	ALA	2.6
1	D	516	VAL	2.6
1	B	305	TYR	2.6
1	B	849	PRO	2.6
1	D	201	TYR	2.6
1	D	198	LEU	2.6
1	B	793	VAL	2.6
1	B	731	GLU	2.6
1	B	507	ASN	2.6
1	B	302	LYS	2.5
1	B	120	PRO	2.5
1	D	490	LEU	2.5
1	D	101	ILE	2.5
1	D	783	SER	2.5
1	B	152	LEU	2.5
1	B	848	TRP	2.5
1	B	531	LYS	2.5
1	D	2	LYS	2.5
1	D	804	HIS	2.5
1	C	301	GLY	2.5
1	A	514	LEU	2.4
1	B	542	LEU	2.4
1	B	805	ILE	2.4
1	B	808	ILE	2.4
1	C	530	ILE	2.4
1	D	183	ILE	2.4
1	B	778	SER	2.4
1	B	841	PHE	2.4
1	D	133	ILE	2.4
1	D	155	PRO	2.4
1	D	811	TYR	2.4
1	D	115	ILE	2.4
1	D	269	SER	2.4
1	D	625	ILE	2.4
1	D	799	PRO	2.4
1	B	842	GLY	2.4
1	D	510	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	859	LYS	2.4
1	D	277	TYR	2.4
1	B	290	LEU	2.4
1	C	303	LEU	2.4
1	D	857	LEU	2.4
1	D	157	GLY	2.3
1	D	520	PHE	2.3
1	B	168	ALA	2.3
1	B	314	GLU	2.3
1	B	820	ASP	2.3
1	A	503	LEU	2.3
1	D	557	ILE	2.3
1	C	506	PRO	2.3
1	B	510	VAL	2.3
1	D	174	GLY	2.3
1	C	514	LEU	2.3
1	B	498	ILE	2.3
1	D	530	ILE	2.3
1	B	824	VAL	2.3
1	B	787	ASN	2.3
1	D	16	PHE	2.3
1	B	164	ILE	2.3
1	B	543	PHE	2.2
1	D	282	PHE	2.2
1	A	535	ALA	2.2
1	D	93	LEU	2.2
1	D	212	ILE	2.2
1	D	148	VAL	2.2
1	D	824	VAL	2.2
1	D	288	TYR	2.2
1	D	518	TYR	2.2
1	A	903	PHE	2.2
1	D	123	PHE	2.2
1	D	479	PHE	2.2
1	D	242	LEU	2.2
1	D	136	ILE	2.2
1	D	140	ASP	2.2
1	B	791	TYR	2.2
1	B	129	ALA	2.2
1	C	498	ILE	2.2
1	C	155	PRO	2.2
1	D	205	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	520	PHE	2.2
1	C	170	LEU	2.2
1	B	535	ALA	2.2
1	D	494	ARG	2.2
1	D	270	VAL	2.2
1	B	737	THR	2.2
1	D	541	MET	2.2
1	D	496	GLY	2.2
1	A	497	GLU	2.2
1	D	545	ALA	2.2
1	B	333	GLN	2.1
1	B	308	PRO	2.1
1	B	130	LYS	2.1
1	B	496	GLY	2.1
1	B	160	GLU	2.1
1	D	9	GLU	2.1
1	D	172	GLU	2.1
1	D	1	MET	2.1
1	D	102	LYS	2.1
1	B	852	THR	2.1
1	D	214	THR	2.1
1	B	508	LEU	2.1
1	B	127	SER	2.1
1	D	509	SER	2.1
1	B	300	VAL	2.1
1	B	522	PHE	2.1
1	D	114	ASP	2.1
1	D	803	PHE	2.1
1	D	431	ALA	2.1
1	B	128	GLN	2.1
1	D	8	VAL	2.1
1	D	793	VAL	2.1
1	B	124	PRO	2.1
1	D	513	PRO	2.1
3	H	113	DC	2.1
1	B	843	ASP	2.1
1	D	28	THR	2.1
1	D	785	ALA	2.1
1	D	391	TYR	2.1
1	B	195	LYS	2.0
1	D	141	SER	2.0
1	D	529	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	179	PRO	2.0
1	B	170	LEU	2.0
1	B	835	LEU	2.0
1	B	860	ASP	2.0
1	B	181	GLU	2.0
1	D	177	GLU	2.0
1	D	501	GLU	2.0
2	E	5	DG	2.0
1	B	119	SER	2.0
1	B	155	PRO	2.0
1	B	306	ASP	2.0
1	D	304	LYS	2.0
1	D	527	LYS	2.0
1	D	250	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CTG	I	4	22/23	0.61	0.16	114,118,119,119	0

6.3 Carbohydrates [i](#)

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.