



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 3E0D / pdb_00003e0d
Title : Insights into the Replisome from the Crystal Structure of the Ternary Complex of the Eubacterial DNA Polymerase III alpha-subunit
Authors : Wing, R.A.; Bailey, S.; Steitz, T.A.
Deposited on : 2008-07-31
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

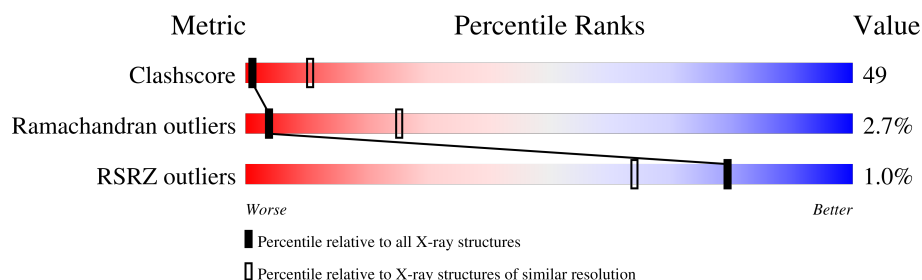
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

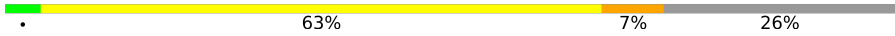
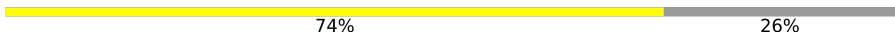
The reported resolution of this entry is 4.60 Å.

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))
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	C	27	
1	E	27	
2	D	21	
2	F	21	
3	A	1220	
3	B	1220	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DOC	D	21	-	-	X	-
2	DOC	F	21	-	-	X	-
5	DTP	A	1222	-	-	X	-
5	DTP	B	1222	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19982 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 DNA chain called DNA substrate template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			
1	E	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			

- Molecule 2 is a DNA chain called DNA substrate primer strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			
2	F	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			

- Molecule 3 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			
3	B	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASN	ASP	engineered mutation	UNP Q9XDH5
A	212	ASN	ASP	engineered mutation	UNP Q9XDH5
A	539	PHE	ILE	engineered mutation	UNP Q9XDH5
A	540	GLU	GLN	engineered mutation	UNP Q9XDH5
A	541	ALA	VAL	engineered mutation	UNP Q9XDH5
A	542	GLU	VAL	engineered mutation	UNP Q9XDH5
B	20	ASN	ASP	engineered mutation	UNP Q9XDH5
B	212	ASN	ASP	engineered mutation	UNP Q9XDH5

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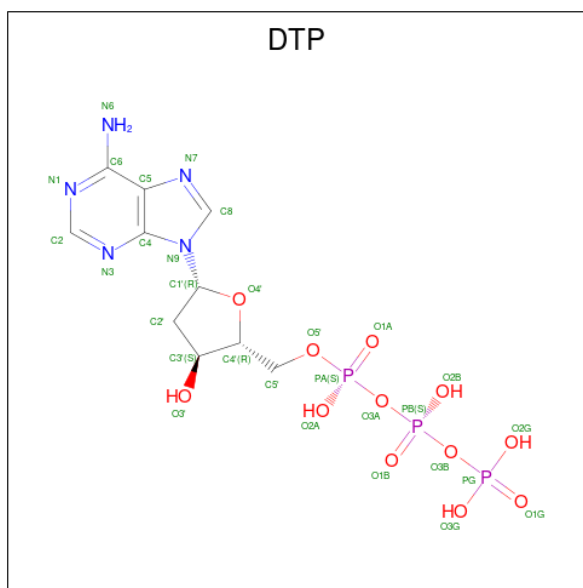
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Chain	Residue	Modelled	Actual	Comment	Reference
B	539	PHE	ILE	engineered mutation	UNP Q9XDH5
B	540	GLU	GLN	engineered mutation	UNP Q9XDH5
B	541	ALA	VAL	engineered mutation	UNP Q9XDH5
B	542	GLU	VAL	engineered mutation	UNP Q9XDH5

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

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

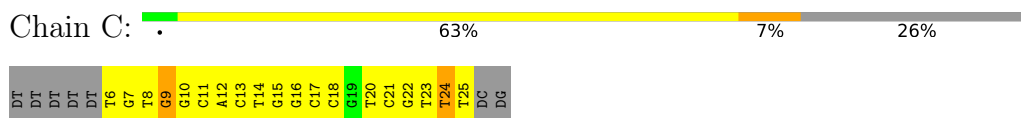


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 30 10 5 12 3	0	0
5	B	1	Total C N O P 30 10 5 12 3	0	0

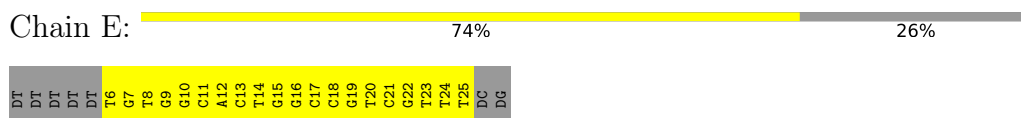
3 Residue-property plots

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.

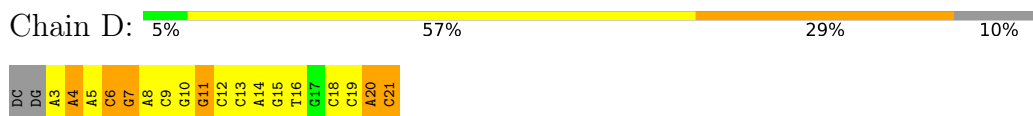
- Molecule 1: DNA substrate template strand



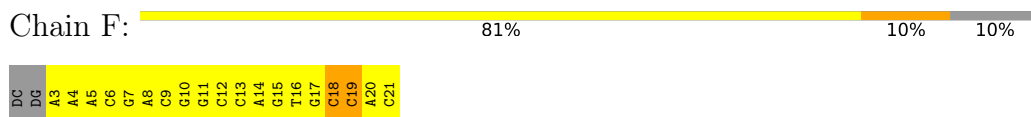
- Molecule 1: DNA substrate template strand



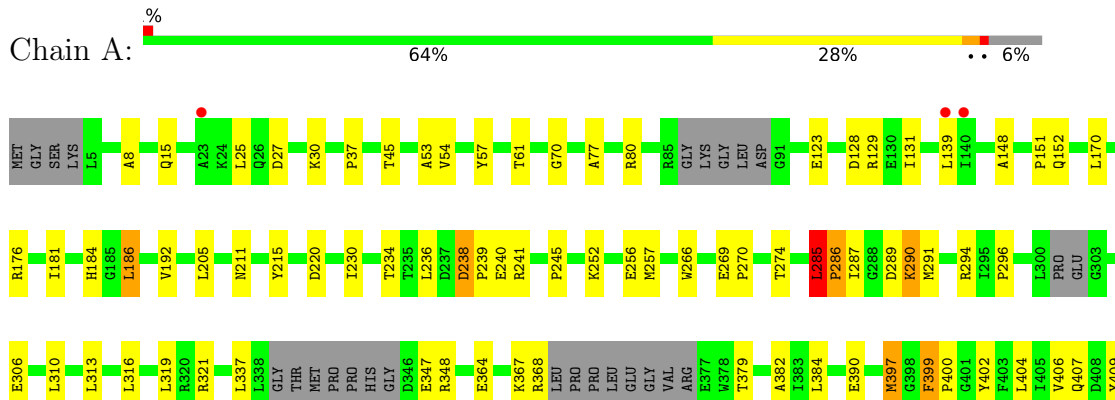
- Molecule 2: DNA substrate primer strand



- Molecule 2: DNA substrate primer strand



- Molecule 3: DNA polymerase III subunit alpha



Y1181	G1182	E1183	A1184	A1185	L1186	G1187	L1188	L1189	E1190	A1191	E1192	G1193	Y1194	P1200	D1201	R1202	F1205	LEU	GLN	GLY	ASN	GLY	GLY	GLY	PRO	VAL	VAL	PRO	PHE																						
GLY	VAL	SER	PRO	LYS	LEU	K1094	E1095	D1096	V1101	L1102	V1105	E1106	LYS	GLY	GLU	GLU	LEU	R1112	V1113	V1118	W1119	E1123	V1124	L1125	E1126	A1127	P1128	K1129	L1140	D1141	E1142	K1143	G1144	VAL	A1146	R1147	L1152	L1159	R1164	F1169	G1170	E1171	A1172	L1173	L1176	R1177	E1178	V1179	R1180		
V1015	L1016	R1017	Y1018	P1019	G1020	L1021	R1022	E1023	S1026	I1029	E1034	F1035	V1036	R1037	E1038	L1039	P1040	G1041	K1042	P1043	L1046	M1050	E1053	V1054	VAL	ARG	LYS	PRO	THR	ARG	SER	GLY	GLY	MET	ALA	R1067	F1068	T1069	L1070	S1071	D1072	E1073	T1074	V1080	VAL	PHE	GLY	ARG	ALA	TYR	GLU
A863	L864	G865	I866	P867	V868	V873	D879	F880	F889	K895	N896	V897	F915	D920	K923	R924	R933	L938	A943	A951	R972	G974	L975	V976	G977	V982	S991	P992	L993	D994	E995	I996	L999	K1003	E1004	A1005	I1008	G1012	H1013	P1014											
H704	I705	P706	T707	Y708	I709	R710	R711	H712	H713	G714	Q715	E716	F717	V718	H725	A726	E727	R731	E736	I740	P741	V742	Y743	Q744	E745	Q746	I747	M748	S752	Y757	S758	L759	G760	D763	L764	L765	R766	R767	A768	M769	R773	V774	E775	E776	M777	Q778	K779	H780	R781	V785	
G604	D605	K606	G607	A608	V609	L612	G613	L614	L615	K616	K617	D618	G621	L622	R623	T624	L625	T626	F627	E630	E637	S638	K639	P653	K654	E657	S660	R661	G662	K665	G666	V667	E671	M675	V679	R680	K683	S695	L696	Y697	R698	P699	G700	P701	M702	E703					

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	149.55Å 149.55Å 163.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.60 50.00 – 4.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.60) 99.7 (50.00-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 4.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.287 , 0.271 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	215.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 485.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19982	wwPDB-VP
Average B, all atoms (Å ²)	233.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: DOC, CA, DTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	1.70	1/454 (0.2%)	0.94	2/700 (0.3%)
1	E	0.45	0/454	0.85	0/700
2	D	1.38	1/413 (0.2%)	1.11	5/635 (0.8%)
2	F	0.49	0/413	0.85	2/635 (0.3%)
3	A	0.94	13/9348 (0.1%)	1.56	30/12615 (0.2%)
3	B	1.07	15/9346 (0.2%)	1.33	29/12608 (0.2%)
All	All	1.02	30/20428 (0.1%)	1.41	68/27893 (0.2%)

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	D	0	3
3	A	3	8
3	B	4	11
All	All	7	22

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	567	GLY	C-N	48.31	1.99	1.33
3	B	397	MET	C-N	45.64	1.86	1.33
3	A	713	HIS	C-N	42.31	1.75	1.33
3	B	713	HIS	C-N	41.85	1.94	1.33
3	B	491	GLN	C-N	40.27	1.88	1.33
1	C	24	DT	O3'-P	35.11	2.13	1.61
3	B	1026	SER	C-N	-32.30	0.89	1.33
3	A	699	PRO	C-N	27.47	1.74	1.33
3	B	621	GLY	C-N	-26.70	0.96	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	DA	O3'-P	23.42	1.96	1.61
3	A	621	GLY	C-N	-16.44	1.09	1.33
3	B	1127	ALA	C-N	-16.23	0.95	1.33
3	B	834	HIS	C-N	-15.22	1.02	1.33
3	A	1127	ALA	C-N	14.04	1.66	1.33
3	B	538	ALA	N-CA	11.81	1.61	1.46
3	A	538	ALA	N-CA	11.74	1.61	1.46
3	B	495	PHE	C-N	10.67	1.49	1.33
3	A	285	LEU	C-N	-10.40	1.09	1.33
3	A	397	MET	C-N	9.63	1.44	1.33
3	A	549	MET	C-N	8.59	1.45	1.33
3	B	549	MET	C-N	8.54	1.45	1.33
3	A	835	TYR	C-N	8.54	1.53	1.33
3	B	538	ALA	CA-CB	-7.93	1.40	1.53
3	A	538	ALA	CA-CB	-7.91	1.40	1.53
3	B	866	ILE	CA-C	7.05	1.60	1.52
3	B	533	LYS	C-O	6.21	1.32	1.23
3	A	533	LYS	C-O	6.10	1.32	1.23
3	A	536	GLN	CG-CD	5.65	1.66	1.52
3	B	536	GLN	CG-CD	5.62	1.66	1.52
3	B	866	ILE	N-CA	5.05	1.52	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	835	TYR	CA-C-N	-62.54	41.67	119.84
3	A	835	TYR	C-N-CA	-62.54	41.67	119.84
3	B	495	PHE	O-C-N	-59.68	43.21	122.59
3	A	699	PRO	CA-C-N	-53.11	38.49	121.87
3	A	699	PRO	C-N-CA	-53.11	38.49	121.87
3	B	1127	ALA	CA-C-N	-49.60	57.84	119.84
3	B	1127	ALA	C-N-CA	-49.60	57.84	119.84
3	A	1127	ALA	O-C-N	-46.27	68.11	121.32
3	B	835	TYR	CA-C-N	-35.33	75.68	119.84
3	B	835	TYR	C-N-CA	-35.33	75.68	119.84
3	A	495	PHE	CA-C-N	-29.91	62.79	121.41
3	A	495	PHE	C-N-CA	-29.91	62.79	121.41
3	A	1127	ALA	CA-C-N	22.34	147.76	119.84
3	A	1127	ALA	C-N-CA	22.34	147.76	119.84
3	A	699	PRO	O-C-N	21.45	151.59	122.64
3	A	835	TYR	O-C-N	-21.08	107.09	121.85
3	A	1127	ALA	C-N-CD	-16.99	55.35	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	491	GLN	O-C-N	-15.80	103.66	122.46
3	A	397	MET	O-C-N	15.53	143.89	122.46
3	B	834	HIS	O-C-N	-15.08	102.28	122.49
3	A	495	PHE	O-C-N	-15.04	94.03	121.70
3	A	285	LEU	CA-C-N	-14.91	101.20	119.84
3	A	285	LEU	C-N-CA	-14.91	101.20	119.84
3	B	1026	SER	O-C-N	-12.70	105.70	122.59
3	A	397	MET	CA-C-N	-10.92	102.44	121.00
3	A	397	MET	C-N-CA	-10.92	102.44	121.00
3	B	495	PHE	CA-C-N	-10.90	100.05	121.41
3	B	495	PHE	C-N-CA	-10.90	100.05	121.41
3	A	567	GLY	O-C-N	-10.60	108.92	122.70
3	B	491	GLN	CA-C-N	-10.34	103.36	121.97
3	B	491	GLN	C-N-CA	-10.34	103.36	121.97
1	C	24	DT	P-O3'-C3'	-10.22	104.86	120.20
3	A	567	GLY	CA-C-N	-10.07	105.00	123.03
3	A	567	GLY	C-N-CA	-10.07	105.00	123.03
3	B	1013	HIS	C-N-CD	-8.96	88.28	125.00
3	B	865	GLY	N-CA-C	8.82	124.06	111.00
3	B	1127	ALA	O-C-N	8.60	131.21	121.32
2	D	3	DA	O5'-C5'-C4'	8.25	123.17	110.80
3	B	1127	ALA	C-N-CD	8.24	158.78	125.00
3	A	713	HIS	CA-C-N	8.12	132.36	120.11
3	A	713	HIS	C-N-CA	8.12	132.36	120.11
3	A	621	GLY	O-C-N	-7.86	112.49	122.70
3	B	397	MET	CA-C-N	7.84	134.33	121.00
3	B	397	MET	C-N-CA	7.84	134.33	121.00
3	B	834	HIS	CA-C-N	7.34	139.70	121.80
3	B	834	HIS	C-N-CA	7.34	139.70	121.80
3	B	835	TYR	O-C-N	7.27	129.68	121.32
2	D	3	DA	P-O3'-C3'	6.98	130.67	120.20
3	A	895	LYS	N-CA-C	6.72	118.40	111.14
3	B	895	LYS	N-CA-C	6.70	118.37	111.14
2	D	3	DA	O3'-P-O5'	-6.42	94.37	104.00
3	A	184	HIS	N-CA-C	-6.02	101.28	109.95
3	B	538	ALA	N-CA-C	6.00	123.57	110.80
3	A	538	ALA	N-CA-C	5.98	123.53	110.80
3	B	184	HIS	N-CA-C	-5.97	101.35	109.95
3	B	397	MET	O-C-N	-5.85	113.88	122.43
3	B	1126	GLU	N-CA-C	5.77	115.64	108.19
2	D	4	DA	C2'-C3'-O3'	5.77	120.15	111.50
1	C	9	DG	C5'-C4'-C3'	-5.77	106.25	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1013	HIS	C-N-CD	-5.75	101.44	125.00
3	B	866	ILE	N-CA-C	5.66	121.11	108.88
3	A	186	LEU	N-CA-C	5.53	117.45	109.48
3	B	186	LEU	N-CA-C	5.46	117.35	109.48
2	D	6	DC	OP1-P-O3'	5.36	124.06	108.00
2	F	18	DC	O3'-P-O5'	5.27	111.90	104.00
3	A	123	GLU	N-CA-C	-5.15	107.06	113.55
2	F	19	DC	N1-C1'-C2'	5.14	121.21	113.50
3	B	123	GLU	N-CA-C	-5.12	107.09	113.55

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	538	ALA	CA
3	A	1013	HIS	CA
3	A	1120	THR	CB
3	B	538	ALA	CA
3	B	866	ILE	CA
3	B	1125	LEU	CA
3	B	1126	GLU	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1012	GLY	Peptide
3	A	1120	THR	Peptide
3	A	1128	PRO	Peptide
3	A	1130	ALA	Peptide
3	A	285	LEU	Mainchain
3	A	337	LEU	Mainchain
3	A	495	PHE	Mainchain
3	A	835	TYR	Mainchain
3	B	1012	GLY	Peptide
3	B	1013	HIS	Peptide
3	B	1026	SER	Mainchain
3	B	1124	VAL	Peptide
3	B	1127	ALA	Mainchain
3	B	337	LEU	Mainchain
3	B	495	PHE	Mainchain
3	B	835	TYR	Mainchain,Peptide
3	B	864	LEU	Peptide
3	B	866	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	D	11	DG	Sidechain
2	D	20	DA	Sidechain
2	D	7	DG	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	C	407	0	230	199	0
1	E	407	0	229	139	0
2	D	385	0	212	143	1
2	F	385	0	212	79	0
3	A	9168	0	9186	869	33
3	B	9168	0	9182	808	35
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	30	0	12	24	0
5	B	30	0	11	14	0
All	All	19982	0	19274	1922	36

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 49.

All (1922) 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)
3:A:1013:HIS:CE1	3:A:1073:GLU:HB3	1.26	1.68
3:A:858:ILE:HD11	3:A:889:PHE:CZ	1.24	1.65
3:A:844:LEU:HB3	3:A:880:PHE:CE1	1.24	1.64
3:B:831:VAL:HG12	3:B:839:PHE:CD1	1.14	1.63
3:B:832:LYS:HB2	3:B:839:PHE:CE2	1.26	1.63
3:A:844:LEU:HB3	3:A:880:PHE:CD1	1.20	1.62
3:A:855:ALA:HB2	3:A:1008:ILE:CG2	1.18	1.62
3:A:855:ALA:CB	3:A:1008:ILE:CG2	1.75	1.61
3:B:831:VAL:CG1	3:B:839:PHE:HD1	1.01	1.60
3:A:855:ALA:CB	3:A:1008:ILE:HG22	1.27	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:546:ARG:CZ	3:A:547:ALA:HB2	1.36	1.56
3:B:54:VAL:HG23	3:B:604:TYR:CZ	1.34	1.56
3:B:491:GLN:HB2	3:B:574:VAL:CG1	1.14	1.55
3:A:574:VAL:CG2	3:A:601:VAL:HG22	1.32	1.55
3:B:996:ILE:HD12	3:B:1017:ARG:CD	1.35	1.55
1:C:8:DT:C5'	3:A:622:LEU:HD23	1.10	1.55
3:B:546:ARG:CZ	3:B:547:ALA:HB2	1.34	1.54
3:A:574:VAL:CG2	3:A:601:VAL:CG2	1.79	1.52
3:B:492:ILE:HG13	3:B:580:VAL:CG2	1.35	1.52
1:C:8:DT:H5''	3:A:622:LEU:CD2	1.38	1.51
3:A:575:HIS:CD2	3:A:578:GLY:N	1.78	1.51
3:A:855:ALA:CA	3:A:1008:ILE:HG21	1.33	1.51
2:F:21:DOC:H2''	3:B:424:ARG:NH1	1.22	1.51
3:B:491:GLN:CB	3:B:574:VAL:CG1	1.87	1.51
3:B:574:VAL:HG22	3:B:601:VAL:CG2	1.40	1.50
3:A:844:LEU:HD22	3:A:880:PHE:CZ	1.45	1.50
3:A:1013:HIS:H	3:A:1014:PRO:CD	1.06	1.49
3:A:858:ILE:CD1	3:A:889:PHE:HZ	1.25	1.48
3:B:996:ILE:CD1	3:B:1017:ARG:HD3	1.42	1.48
2:D:21:DOC:H2''	3:A:424:ARG:NH1	1.18	1.47
3:B:996:ILE:CG1	3:B:1017:ARG:HD2	1.44	1.46
1:E:14:DT:P	3:B:509:ARG:HH12	1.38	1.45
3:A:713:HIS:C	3:A:714:GLY:N	1.75	1.44
3:B:1128:PRO:HG3	3:B:1129:LYS:CE	1.10	1.44
3:A:774:VAL:CB	3:B:778:GLN:HG2	1.46	1.43
3:A:844:LEU:CB	3:A:880:PHE:CD1	2.02	1.41
3:A:858:ILE:CD1	3:A:889:PHE:CZ	1.99	1.41
3:B:1128:PRO:CG	3:B:1129:LYS:HE3	1.22	1.41
3:A:1013:HIS:ND1	3:A:1073:GLU:HB3	1.36	1.40
3:B:54:VAL:CG2	3:B:604:TYR:CE1	2.02	1.39
3:B:996:ILE:CD1	3:B:1017:ARG:CD	1.92	1.39
3:A:574:VAL:HG22	3:A:601:VAL:CG2	0.90	1.38
3:A:996:ILE:HD11	3:A:1018:TYR:CE2	1.58	1.38
3:B:832:LYS:CB	3:B:839:PHE:CE2	2.07	1.38
3:B:492:ILE:CG1	3:B:580:VAL:HG22	1.53	1.37
1:C:8:DT:C5'	3:A:622:LEU:CD2	1.96	1.37
3:A:458:ARG:CZ	3:A:764:LEU:CD2	2.01	1.36
3:A:575:HIS:CD2	3:A:578:GLY:H	1.37	1.36
3:A:458:ARG:NH1	3:A:764:LEU:HD22	1.37	1.34
3:A:458:ARG:CZ	3:A:764:LEU:HD22	1.57	1.34
3:A:523:LYS:HD2	3:A:1094:LYS:NZ	1.36	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:458:ARG:NH1	3:A:764:LEU:CD2	1.92	1.33
3:B:397:MET:C	3:B:398:GLY:N	1.86	1.33
3:A:575:HIS:HD2	3:A:578:GLY:N	1.09	1.32
3:B:1046:LEU:HD21	3:B:1202:ARG:NH2	1.40	1.32
3:A:832:LYS:HB2	3:A:839:PHE:CE2	1.64	1.31
3:B:710:ARG:NH1	3:B:716:GLU:OE1	1.58	1.31
3:B:491:GLN:C	3:B:492:ILE:N	1.88	1.31
1:C:9:DG:C4'	3:A:621:GLY:H	1.44	1.31
3:B:699:PRO:HA	3:B:700:GLY:N	1.43	1.31
3:B:844:LEU:HB3	3:B:880:PHE:CD1	1.66	1.30
3:A:1027:CYS:SG	3:A:1031:GLU:HB2	1.72	1.30
3:A:851:SER:OG	3:A:895:LYS:CE	1.80	1.29
1:E:14:DT:OP1	3:B:509:ARG:NH1	1.65	1.29
3:A:744:GLN:N	3:A:813:PHE:N	1.80	1.29
3:A:744:GLN:H	3:A:813:PHE:N	1.26	1.29
1:C:8:DT:C3'	3:A:623:ARG:H	1.46	1.29
3:A:774:VAL:HG23	3:B:778:GLN:CB	1.63	1.28
3:A:230:ILE:CD1	3:A:565:LEU:CD1	2.11	1.28
3:A:844:LEU:CB	3:A:880:PHE:CE1	2.13	1.28
3:A:1013:HIS:CE1	3:A:1073:GLU:CB	2.18	1.27
1:C:8:DT:P	3:A:623:ARG:HB2	1.73	1.26
3:B:696:LEU:CD2	3:B:742:VAL:HG22	1.66	1.26
1:C:9:DG:H4'	3:A:621:GLY:N	1.49	1.25
3:B:543:PRO:O	3:B:546:ARG:HD2	1.28	1.25
3:B:996:ILE:CG1	3:B:1017:ARG:CD	2.13	1.25
3:B:1046:LEU:CD2	3:B:1202:ARG:HH21	1.50	1.25
3:B:321:ARG:HH22	3:B:440:ASN:ND2	1.34	1.24
3:B:713:HIS:C	3:B:714:GLY:N	1.94	1.24
3:B:699:PRO:C	3:B:700:GLY:HA3	1.63	1.24
1:E:14:DT:H4'	3:B:509:ARG:NH2	1.50	1.24
3:A:665:LYS:CB	3:A:860:ASP:OD2	1.85	1.24
3:A:665:LYS:HB3	3:A:860:ASP:OD2	1.06	1.23
3:A:543:PRO:O	3:A:546:ARG:HD2	1.35	1.22
3:B:832:LYS:HB2	3:B:839:PHE:CZ	1.73	1.22
3:A:696:LEU:HD21	3:A:742:VAL:CG2	1.67	1.22
3:B:54:VAL:HG21	3:B:604:TYR:CE1	1.67	1.22
3:B:848:ARG:NE	3:B:879:ASP:OD2	1.72	1.22
3:B:458:ARG:NH1	3:B:764:LEU:HD22	1.56	1.21
3:A:699:PRO:O	3:A:811:TYR:CD2	1.93	1.21
3:A:774:VAL:N	3:B:778:GLN:CD	1.74	1.21
1:C:8:DT:H4'	3:A:622:LEU:CA	1.70	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1013:HIS:ND1	3:A:1073:GLU:CB	2.02	1.20
3:B:54:VAL:HG23	3:B:604:TYR:CE1	1.69	1.20
1:C:9:DG:N3	3:A:576:ALA:CB	2.05	1.20
3:A:773:ARG:CB	3:B:778:GLN:HE22	1.38	1.20
3:A:567:GLY:C	3:A:568:LEU:N	1.99	1.20
3:A:1013:HIS:N	3:A:1014:PRO:HD2	1.24	1.20
3:B:699:PRO:CA	3:B:700:GLY:N	2.04	1.20
3:A:845:SER:HA	3:A:879:ASP:OD1	1.39	1.20
3:A:1003:LYS:NZ	3:A:1096:ASP:OD1	1.75	1.20
1:E:14:DT:P	3:B:509:ARG:NH1	2.16	1.19
1:C:8:DT:C4'	3:A:622:LEU:HA	1.71	1.19
2:D:21:DOC:H2'	5:A:1222:DTP:O4'	1.36	1.19
1:E:18:DC:OP1	3:B:933:ARG:HB2	1.40	1.19
3:A:455:ASN:HD21	3:A:760:GLY:C	1.47	1.19
3:A:845:SER:OG	3:A:879:ASP:OD2	1.59	1.18
3:A:773:ARG:HG2	3:B:778:GLN:CD	1.66	1.18
3:A:775:GLU:OE1	3:B:781:ARG:NE	1.74	1.18
3:B:744:GLN:H	3:B:813:PHE:C	1.51	1.18
3:A:851:SER:OG	3:A:895:LYS:NZ	1.76	1.18
3:A:697:TYR:CE1	3:A:702:MET:SD	2.37	1.17
3:B:665:LYS:HD3	3:B:860:ASP:CB	1.73	1.17
3:B:699:PRO:C	3:B:700:GLY:CA	2.15	1.17
3:B:54:VAL:CG2	3:B:604:TYR:CZ	2.22	1.17
3:B:707:THR:CG2	3:B:716:GLU:OE2	1.92	1.17
3:A:773:ARG:HG2	3:B:778:GLN:NE2	1.57	1.16
3:B:452:ARG:NH2	3:B:766:ARG:CZ	2.08	1.16
3:B:455:ASN:HD21	3:B:760:GLY:C	1.50	1.16
3:A:1013:HIS:N	3:A:1014:PRO:CD	1.78	1.16
1:E:8:DT:C4'	3:B:622:LEU:HD23	1.76	1.16
3:A:773:ARG:CG	3:B:778:GLN:NE2	2.08	1.16
3:A:1027:CYS:SG	3:A:1031:GLU:CB	2.33	1.16
2:D:21:DOC:C2'	3:A:424:ARG:NH1	2.08	1.15
3:B:714:GLY:O	3:B:715:GLN:HG3	1.44	1.15
3:B:665:LYS:HD3	3:B:860:ASP:HB3	1.25	1.15
3:A:230:ILE:CD1	3:A:565:LEU:HD11	1.74	1.15
1:C:10:DG:C4'	3:A:576:ALA:HA	1.76	1.15
1:C:14:DT:O3'	3:A:509:ARG:NH1	1.80	1.15
3:A:634:ILE:CG2	3:A:838:GLU:HB3	1.74	1.15
2:F:21:DOC:C2'	3:B:424:ARG:NH1	2.09	1.14
2:D:21:DOC:C2'	3:A:424:ARG:HH12	1.60	1.14
3:A:1129:LYS:HA	3:A:1199:VAL:C	1.71	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:699:PRO:C	3:B:700:GLY:N	2.06	1.14
3:B:699:PRO:C	3:B:701:PRO:HD2	1.73	1.13
3:B:744:GLN:N	3:B:813:PHE:N	1.96	1.13
3:A:698:ARG:O	3:A:701:PRO:CD	1.96	1.13
3:A:1129:LYS:HA	3:A:1200:PRO:CA	1.77	1.13
3:B:996:ILE:HG13	3:B:1017:ARG:CB	1.77	1.13
3:B:1128:PRO:CG	3:B:1129:LYS:CE	1.88	1.13
3:A:866:ILE:CG2	3:A:867:PRO:HD2	1.79	1.13
3:A:455:ASN:HD21	3:A:760:GLY:CA	1.61	1.12
3:A:1130:ALA:N	3:A:1199:VAL:O	1.80	1.13
3:B:831:VAL:CG1	3:B:839:PHE:CD1	1.89	1.12
3:A:1129:LYS:HA	3:A:1199:VAL:O	1.50	1.12
3:B:574:VAL:HG22	3:B:601:VAL:HG22	1.21	1.12
3:B:707:THR:HG23	3:B:716:GLU:OE2	1.47	1.12
1:C:8:DT:H3'	3:A:623:ARG:H	1.10	1.12
3:B:844:LEU:HD22	3:B:880:PHE:CE1	1.84	1.12
3:A:575:HIS:CG	3:A:578:GLY:H	1.68	1.12
3:B:831:VAL:HB	3:B:839:PHE:CE1	1.84	1.12
3:B:996:ILE:HG13	3:B:1017:ARG:CG	1.80	1.12
2:D:9:DC:H1'	2:D:10:DG:H5''	1.24	1.11
2:F:20:DA:H2''	2:F:21:DOC:H5'	1.30	1.11
3:B:704:HIS:CD2	3:B:808:PHE:HE2	1.68	1.11
3:A:492:ILE:HD12	3:A:616:LYS:HG3	1.27	1.11
3:A:1024:VAL:CG2	3:A:1200:PRO:HD2	1.79	1.11
3:A:523:LYS:CD	3:A:1094:LYS:HZ3	1.63	1.11
3:A:627:PHE:HE1	3:A:843:LEU:N	1.48	1.11
3:A:696:LEU:CD2	3:A:742:VAL:HG22	1.79	1.11
3:B:665:LYS:CD	3:B:860:ASP:HB3	1.81	1.11
3:B:696:LEU:HD21	3:B:742:VAL:CG2	1.79	1.10
3:B:812:GLY:C	3:B:813:PHE:HA	1.74	1.10
3:B:452:ARG:NH2	3:B:766:ARG:NH2	2.00	1.10
3:B:704:HIS:NE2	3:B:808:PHE:CZ	2.18	1.10
2:D:20:DA:H2''	2:D:21:DOC:H5'	1.25	1.10
3:A:779:LYS:NZ	3:B:774:VAL:HA	1.67	1.10
3:B:491:GLN:CB	3:B:574:VAL:HG12	1.61	1.10
3:B:546:ARG:CZ	3:B:547:ALA:CB	2.30	1.10
3:B:491:GLN:HB3	3:B:574:VAL:HG12	1.25	1.09
3:B:546:ARG:HD3	3:B:547:ALA:N	1.65	1.09
3:B:996:ILE:CB	3:B:1017:ARG:HD2	1.81	1.09
3:B:701:PRO:HD3	3:B:811:TYR:CD1	1.86	1.09
1:E:8:DT:H4'	3:B:622:LEU:HD23	1.23	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:574:VAL:HG22	3:A:601:VAL:HG21	1.18	1.09
3:A:230:ILE:HD11	3:A:565:LEU:HD11	1.33	1.09
3:A:1120:THR:O	3:A:1124:VAL:HG23	1.49	1.08
3:A:458:ARG:CZ	3:A:764:LEU:HD21	1.77	1.08
3:A:776:GLU:HG3	3:B:775:GLU:HG3	1.35	1.08
3:A:844:LEU:CD2	3:A:880:PHE:CZ	2.36	1.08
3:A:1129:LYS:CA	3:A:1199:VAL:O	2.01	1.08
3:B:493:GLY:H	3:B:602:THR:HB	1.17	1.08
3:A:523:LYS:CD	3:A:1094:LYS:NZ	2.16	1.08
3:B:574:VAL:HG22	3:B:601:VAL:HG21	1.24	1.08
1:C:9:DG:H3'	3:A:621:GLY:HA3	1.29	1.08
1:C:14:DT:N3	2:D:14:DA:N1	2.02	1.08
1:E:13:DC:H2''	1:E:14:DT:H5''	1.22	1.08
3:A:496:GLY:O	3:A:569:ASN:HA	1.53	1.08
3:A:866:ILE:HG23	3:A:867:PRO:CD	1.83	1.08
3:A:546:ARG:CZ	3:A:547:ALA:CB	2.31	1.07
3:A:994:ASP:HB2	3:A:1017:ARG:CZ	1.84	1.07
3:B:665:LYS:HZ3	3:B:864:LEU:HD13	1.12	1.07
3:A:455:ASN:ND2	3:A:760:GLY:CA	2.16	1.07
3:B:999:LEU:HD11	3:B:1013:HIS:N	1.70	1.07
3:A:230:ILE:CD1	3:A:565:LEU:HD13	1.84	1.07
3:A:851:SER:OG	3:A:895:LYS:HE2	1.40	1.07
1:C:15:DG:C2	2:D:14:DA:C2	2.42	1.06
1:E:10:DG:O4'	3:B:576:ALA:HB2	1.55	1.06
2:F:19:DC:H5''	3:B:531:LYS:NZ	1.68	1.06
3:A:855:ALA:HB1	3:A:1008:ILE:HG22	1.34	1.06
1:C:24:DT:O3'	1:C:25:DT:P	2.13	1.06
3:A:424:ARG:NH1	5:A:1222:DTP:H4'	1.71	1.06
3:A:844:LEU:HD22	3:A:880:PHE:CE1	1.90	1.06
3:B:866:ILE:CG2	3:B:867:PRO:N	2.19	1.06
3:A:773:ARG:HB3	3:B:778:GLN:HE22	0.92	1.06
3:A:855:ALA:CA	3:A:1008:ILE:CG2	2.14	1.06
3:B:999:LEU:CD1	3:B:1013:HIS:CA	2.10	1.06
1:E:8:DT:H1'	1:E:9:DG:O5'	1.56	1.05
2:D:21:DOC:H3'1	5:A:1222:DTP:H5'1	1.37	1.05
3:A:698:ARG:O	3:A:701:PRO:HD2	1.55	1.05
3:B:455:ASN:HD21	3:B:760:GLY:CA	1.69	1.05
3:B:704:HIS:NE2	3:B:808:PHE:CE2	2.24	1.05
3:A:1129:LYS:C	3:A:1199:VAL:O	1.99	1.05
3:B:1035:PHE:HA	3:B:1170:GLY:HA3	1.33	1.05
3:A:996:ILE:HD11	3:A:1018:TYR:HE2	0.92	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:996:ILE:HD11	3:B:1017:ARG:HB3	1.34	1.05
3:A:773:ARG:CB	3:B:778:GLN:NE2	1.99	1.04
3:B:671:GLU:OE2	3:B:853:LYS:NZ	1.91	1.04
3:A:1013:HIS:H	3:A:1014:PRO:HD3	0.91	1.04
3:B:743:TYR:C	3:B:813:PHE:N	2.15	1.04
1:C:8:DT:C4'	3:A:622:LEU:HD23	1.88	1.04
3:A:523:LYS:HD3	3:A:1054:VAL:HG13	1.39	1.04
3:B:1035:PHE:CE1	3:B:1171:GLU:O	2.11	1.04
3:A:492:ILE:HG13	3:A:580:VAL:HG22	1.35	1.03
3:A:535:LEU:HB3	3:A:563:MET:HE2	1.37	1.03
1:E:13:DC:C2'	1:E:14:DT:H5''	1.87	1.03
3:B:535:LEU:HB3	3:B:563:MET:HE2	1.36	1.03
3:A:230:ILE:HD13	3:A:565:LEU:HD13	1.39	1.03
3:A:457:GLU:OE2	3:A:758:SER:OG	1.75	1.03
3:A:855:ALA:HB2	3:A:1008:ILE:HG23	1.38	1.03
3:A:634:ILE:HG22	3:A:838:GLU:CB	1.89	1.02
3:B:458:ARG:NH1	3:B:764:LEU:CD2	2.22	1.02
3:A:492:ILE:CD1	3:A:616:LYS:HG3	1.87	1.02
3:B:1035:PHE:CE1	3:B:1171:GLU:C	2.37	1.02
3:A:321:ARG:HH22	3:A:440:ASN:ND2	1.57	1.02
3:A:774:VAL:HG23	3:B:778:GLN:HB3	1.05	1.02
3:B:491:GLN:HB2	3:B:574:VAL:HG11	1.38	1.02
1:C:9:DG:C4'	3:A:621:GLY:N	2.12	1.02
3:B:574:VAL:CG2	3:B:601:VAL:CG2	2.36	1.02
1:E:13:DC:H2''	1:E:14:DT:C5'	1.89	1.02
1:E:14:DT:C4'	3:B:509:ARG:HH22	1.73	1.02
3:A:774:VAL:CG2	3:B:778:GLN:CB	2.38	1.02
3:B:817:HIS:CE1	5:B:1222:DTP:H2'1	1.90	1.02
1:C:8:DT:C3'	3:A:623:ARG:N	2.23	1.01
1:C:8:DT:OP2	3:A:623:ARG:HB2	1.59	1.01
3:A:1129:LYS:CA	3:A:1200:PRO:HA	1.67	1.01
3:B:447:GLY:H	3:B:815:LYS:NZ	1.58	1.01
3:B:491:GLN:CB	3:B:574:VAL:HG11	1.89	1.01
3:B:704:HIS:CD2	3:B:808:PHE:CE2	2.48	1.01
3:B:1123:GLU:O	3:B:1126:GLU:OE1	1.79	1.01
2:D:21:DOC:H6	2:D:21:DOC:H5''	1.39	1.01
3:A:634:ILE:HG22	3:A:838:GLU:HB3	1.40	1.01
3:A:773:ARG:C	3:B:778:GLN:NE2	2.00	1.01
3:A:455:ASN:OD1	3:A:760:GLY:HA3	1.58	1.01
3:B:996:ILE:HG13	3:B:1017:ARG:HD2	1.41	1.01
3:A:774:VAL:HB	3:B:778:GLN:HG2	1.04	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1028:THR:O	3:A:1031:GLU:N	1.93	1.00
3:B:812:GLY:C	3:B:813:PHE:CA	2.33	1.00
2:D:6:DC:H2''	2:D:7:DG:OP2	1.58	1.00
3:A:234:THR:O	3:A:510:VAL:HG13	1.61	1.00
3:A:523:LYS:HD3	3:A:1054:VAL:CG1	1.92	1.00
3:A:743:TYR:HA	3:A:813:PHE:N	1.77	1.00
3:A:745:GLU:OE1	3:A:813:PHE:O	1.78	1.00
3:A:862:ARG:HE	3:A:868:VAL:HB	1.27	1.00
1:C:8:DT:H1'	1:C:9:DG:O5'	1.60	1.00
3:A:774:VAL:HB	3:B:778:GLN:CG	1.91	1.00
3:A:832:LYS:CB	3:A:839:PHE:CE2	2.45	1.00
3:B:996:ILE:CG1	3:B:1017:ARG:CB	2.39	1.00
3:A:634:ILE:CG2	3:A:838:GLU:CB	2.39	0.99
3:A:774:VAL:CB	3:B:778:GLN:CG	2.40	0.99
3:A:627:PHE:HA	3:A:846:VAL:HG21	1.43	0.99
3:B:1126:GLU:HG3	3:B:1205:PHE:CE2	1.97	0.99
3:A:575:HIS:HB3	3:A:578:GLY:HA3	1.38	0.99
3:A:1046:LEU:HD21	3:A:1202:ARG:HE	1.27	0.99
3:B:996:ILE:HG13	3:B:1017:ARG:CD	1.85	0.99
3:A:779:LYS:HZ2	3:B:774:VAL:HA	1.23	0.99
3:B:832:LYS:HA	3:B:839:PHE:CD2	1.97	0.99
3:B:543:PRO:O	3:B:546:ARG:CD	2.11	0.99
1:C:8:DT:H5'	3:A:622:LEU:CD2	1.88	0.99
3:A:1013:HIS:HD2	3:A:1015:VAL:H	1.00	0.99
1:E:8:DT:H5''	3:B:622:LEU:CD2	1.92	0.98
3:A:496:GLY:O	3:A:569:ASN:CA	2.09	0.98
3:B:455:ASN:ND2	3:B:760:GLY:O	1.96	0.98
3:A:424:ARG:NH1	5:A:1222:DTP:C4'	2.25	0.98
3:B:627:PHE:HE1	3:B:843:LEU:N	1.62	0.98
2:D:21:DOC:C2'	5:A:1222:DTP:O4'	2.12	0.98
3:B:58:LYS:CB	3:B:287:ILE:CD1	2.40	0.98
3:A:546:ARG:NE	3:A:547:ALA:HB2	1.78	0.98
3:A:699:PRO:O	3:A:811:TYR:HD2	1.47	0.98
2:D:9:DC:H1'	2:D:10:DG:C5'	1.93	0.98
3:B:546:ARG:NE	3:B:547:ALA:HB2	1.79	0.98
3:A:458:ARG:NE	3:A:764:LEU:HD21	1.78	0.98
2:D:21:DOC:H6	2:D:21:DOC:C5'	1.93	0.97
3:A:773:ARG:CG	3:B:778:GLN:CD	2.29	0.97
3:B:455:ASN:ND2	3:B:760:GLY:CA	2.26	0.97
3:A:745:GLU:OE2	3:A:814:ASN:ND2	1.97	0.97
3:A:1129:LYS:HA	3:A:1200:PRO:HA	1.38	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:627:PHE:HA	3:B:846:VAL:HG21	1.46	0.97
1:C:11:DC:H4'	3:A:573:SER:HB3	1.45	0.97
3:B:831:VAL:HB	3:B:839:PHE:HE1	1.19	0.97
3:B:999:LEU:CD1	3:B:1013:HIS:N	2.26	0.97
3:A:844:LEU:HD22	3:A:880:PHE:HZ	1.27	0.97
1:C:8:DT:H5'	3:A:622:LEU:HD23	1.38	0.97
3:A:455:ASN:ND2	3:A:760:GLY:HA2	1.80	0.96
3:A:855:ALA:HA	3:A:1008:ILE:CG2	1.88	0.96
2:F:19:DC:H5''	3:B:531:LYS:HZ1	1.24	0.96
3:A:774:VAL:CA	3:B:778:GLN:HG2	1.95	0.96
3:B:999:LEU:HD11	3:B:1013:HIS:H	1.29	0.96
3:A:1129:LYS:HA	3:A:1200:PRO:N	1.80	0.96
3:B:424:ARG:NE	5:B:1222:DTP:H4'	1.81	0.96
3:A:996:ILE:CD1	3:A:1018:TYR:HE2	1.79	0.96
3:B:1035:PHE:CD1	3:B:1171:GLU:N	2.33	0.95
1:E:8:DT:O3'	3:B:623:ARG:N	1.98	0.95
3:B:866:ILE:HG22	3:B:867:PRO:C	1.92	0.95
3:A:539:PHE:HZ	3:A:559:ILE:CG2	1.79	0.95
3:A:634:ILE:HG21	3:A:838:GLU:HB3	1.49	0.95
3:A:574:VAL:CG2	3:A:601:VAL:HG21	1.73	0.95
3:A:866:ILE:HG23	3:A:867:PRO:HD2	0.95	0.95
3:A:496:GLY:O	3:A:569:ASN:CB	2.14	0.95
3:A:775:GLU:CD	3:B:781:ARG:HE	1.74	0.95
3:A:774:VAL:CG2	3:B:778:GLN:HB3	1.95	0.94
3:B:491:GLN:HB2	3:B:574:VAL:HG13	0.95	0.94
1:C:10:DG:H4'	3:A:576:ALA:HA	1.45	0.94
3:A:575:HIS:CD2	3:A:578:GLY:CA	2.50	0.94
3:A:865:GLY:O	3:A:866:ILE:HG13	1.66	0.94
3:B:539:PHE:HZ	3:B:559:ILE:CG2	1.79	0.94
3:A:698:ARG:C	3:A:701:PRO:HD2	1.91	0.94
3:A:776:GLU:CG	3:B:775:GLU:HG3	1.98	0.94
2:F:21:DOC:H2''	3:B:424:ARG:HH12	1.29	0.94
3:A:535:LEU:HD23	3:A:539:PHE:HE1	1.30	0.94
3:A:539:PHE:CZ	3:A:559:ILE:CG2	2.51	0.94
3:A:696:LEU:HG	3:A:742:VAL:CG1	1.96	0.94
3:A:774:VAL:N	3:B:778:GLN:CG	2.31	0.94
3:B:699:PRO:O	3:B:811:TYR:CD1	2.15	0.94
1:C:9:DG:C3'	3:A:621:GLY:HA3	1.97	0.94
3:A:543:PRO:O	3:A:546:ARG:CD	2.16	0.94
3:A:455:ASN:ND2	3:A:760:GLY:O	2.01	0.93
3:B:539:PHE:CZ	3:B:559:ILE:CG2	2.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:999:LEU:HB3	3:B:1014:PRO:CG	1.97	0.93
3:B:711:ARG:HG2	3:B:716:GLU:O	1.68	0.93
3:B:452:ARG:HH22	3:B:766:ARG:NH2	1.63	0.93
3:B:535:LEU:HD23	3:B:539:PHE:HE1	1.31	0.93
1:E:18:DC:P	3:B:933:ARG:HD3	2.09	0.93
3:B:493:GLY:N	3:B:602:THR:HB	1.83	0.93
3:A:1143:LYS:HA	3:A:1147:ARG:HB2	1.50	0.93
3:B:58:LYS:HB2	3:B:287:ILE:CD1	1.98	0.93
3:B:546:ARG:NH1	3:B:547:ALA:HB2	1.83	0.93
3:B:831:VAL:CB	3:B:839:PHE:CD1	2.51	0.93
3:B:447:GLY:N	3:B:815:LYS:HZ2	1.65	0.92
3:A:855:ALA:HA	3:A:1008:ILE:HG21	0.94	0.92
3:B:321:ARG:NH2	3:B:440:ASN:HD21	1.68	0.92
3:A:1026:SER:HB3	3:A:1202:ARG:NH2	1.84	0.92
3:A:844:LEU:CD2	3:A:880:PHE:CE1	2.51	0.92
3:A:696:LEU:HG	3:A:742:VAL:HG13	1.51	0.92
3:A:1013:HIS:CD2	3:A:1015:VAL:HG12	2.05	0.92
3:B:575:HIS:HB3	3:B:578:GLY:HA3	1.48	0.92
1:C:8:DT:OP1	3:A:623:ARG:HB2	1.69	0.92
2:D:5:DA:H2''	2:D:6:DC:OP2	1.68	0.92
3:A:844:LEU:HD13	3:A:880:PHE:CE2	2.05	0.92
3:B:707:THR:HG22	3:B:716:GLU:OE2	1.68	0.92
3:B:54:VAL:HG21	3:B:604:TYR:CD1	2.04	0.92
3:B:831:VAL:HG12	3:B:839:PHE:CG	2.05	0.92
1:E:8:DT:H4'	3:B:622:LEU:CD2	1.99	0.91
3:A:230:ILE:HD11	3:A:565:LEU:CD1	1.90	0.91
3:A:701:PRO:HD3	3:A:811:TYR:HB3	1.52	0.91
3:B:1143:LYS:HA	3:B:1147:ARG:HB2	1.50	0.91
3:A:627:PHE:CA	3:A:846:VAL:HG21	2.00	0.91
3:A:832:LYS:HB2	3:A:839:PHE:CZ	2.04	0.91
3:A:1035:PHE:CD1	3:A:1171:GLU:O	2.23	0.91
3:A:773:ARG:HB3	3:B:778:GLN:NE2	1.74	0.91
3:B:1141:ASP:O	3:B:1143:LYS:N	2.02	0.91
3:B:996:ILE:CD1	3:B:1017:ARG:HB3	1.99	0.91
3:A:397:MET:HE3	3:A:459:VAL:HA	1.52	0.91
3:B:831:VAL:CB	3:B:839:PHE:CE1	2.53	0.91
3:B:862:ARG:HE	3:B:868:VAL:HB	1.36	0.91
3:A:866:ILE:CG2	3:A:867:PRO:CD	2.45	0.91
3:B:321:ARG:NH2	3:B:440:ASN:ND2	2.18	0.91
2:D:21:DOC:H2''	3:A:424:ARG:HH11	1.16	0.91
1:E:8:DT:C5'	3:B:622:LEU:HD23	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1099:LEU:HD22	3:A:1119:TRP:O	1.71	0.90
3:B:848:ARG:HE	3:B:879:ASP:CG	1.79	0.90
3:B:110:VAL:HG11	3:B:587:THR:O	1.71	0.90
1:E:9:DG:H1'	1:E:10:DG:C5'	2.01	0.90
3:B:496:GLY:O	3:B:569:ASN:HA	1.71	0.90
3:A:575:HIS:HB3	3:A:578:GLY:CA	2.00	0.90
3:A:1013:HIS:HE1	3:A:1073:GLU:HB3	1.35	0.90
3:A:321:ARG:HH22	3:A:440:ASN:HD21	1.18	0.90
1:E:17:DC:O3'	3:B:933:ARG:HD3	1.69	0.90
3:A:1024:VAL:HG23	3:A:1200:PRO:HD2	1.51	0.90
3:B:452:ARG:HH21	3:B:766:ARG:CZ	1.81	0.90
2:F:21:DOC:C2'	3:B:424:ARG:HH12	1.81	0.90
3:B:458:ARG:NH2	3:B:764:LEU:HD13	1.87	0.90
3:B:744:GLN:N	3:B:813:PHE:O	2.05	0.90
3:B:1126:GLU:HG3	3:B:1205:PHE:CZ	2.07	0.90
3:A:458:ARG:NH2	3:A:764:LEU:HD13	1.86	0.89
3:A:627:PHE:CZ	3:A:843:LEU:HG	2.06	0.89
1:E:14:DT:O5'	3:B:509:ARG:NH1	2.03	0.89
3:B:110:VAL:HG12	3:B:587:THR:HG22	1.52	0.89
3:A:698:ARG:O	3:A:701:PRO:N	2.06	0.89
1:E:10:DG:H4'	3:B:576:ALA:HA	1.54	0.89
3:A:289:ASP:HB3	3:B:62:ALA:O	1.73	0.89
3:B:58:LYS:HB3	3:B:287:ILE:CD1	2.01	0.89
3:B:866:ILE:HG22	3:B:867:PRO:N	1.84	0.89
3:A:458:ARG:CD	3:A:764:LEU:HD21	2.03	0.89
3:B:428:ALA:HB3	3:B:816:SER:HB2	1.54	0.89
3:A:627:PHE:CE1	3:A:843:LEU:HA	2.07	0.89
3:A:862:ARG:NH2	3:A:1010:VAL:HG13	1.87	0.89
3:B:546:ARG:HD3	3:B:546:ARG:C	1.95	0.89
3:B:665:LYS:NZ	3:B:864:LEU:HD13	1.87	0.89
3:B:999:LEU:HB3	3:B:1014:PRO:HG3	1.55	0.89
3:B:1128:PRO:HG3	3:B:1129:LYS:NZ	1.88	0.89
1:E:14:DT:H4'	3:B:509:ARG:HH22	0.78	0.88
3:B:492:ILE:CD1	3:B:580:VAL:HG22	2.03	0.88
2:D:19:DC:H2'	3:A:531:LYS:NZ	1.87	0.88
3:B:1140:LEU:HD12	3:B:1143:LYS:NZ	1.88	0.88
2:F:20:DA:C2'	2:F:21:DOC:H5'	2.02	0.88
3:B:844:LEU:HD22	3:B:880:PHE:CZ	2.06	0.88
3:A:994:ASP:HB2	3:A:1017:ARG:NH2	1.89	0.88
3:A:492:ILE:HD11	3:A:616:LYS:HB2	1.52	0.88
3:A:696:LEU:CD2	3:A:742:VAL:HG13	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:235:THR:HA	3:B:510:VAL:O	1.72	0.88
3:B:832:LYS:HB2	3:B:839:PHE:HE2	1.27	0.88
3:B:996:ILE:HG13	3:B:1017:ARG:HB2	1.51	0.88
1:C:24:DT:H2''	1:C:25:DT:P	2.14	0.88
3:A:627:PHE:CE1	3:A:843:LEU:N	2.41	0.88
3:A:539:PHE:CZ	3:A:559:ILE:HG21	2.09	0.87
3:B:665:LYS:CD	3:B:860:ASP:CB	2.46	0.87
3:A:996:ILE:HD11	3:A:1018:TYR:CZ	2.09	0.87
3:A:1013:HIS:CD2	3:A:1015:VAL:H	1.92	0.87
3:B:996:ILE:HB	3:B:1017:ARG:HD2	1.55	0.87
3:B:575:HIS:HB3	3:B:578:GLY:CA	2.03	0.87
3:A:851:SER:HG	3:A:895:LYS:HE2	1.36	0.87
3:B:744:GLN:H	3:B:813:PHE:CA	1.87	0.87
3:B:866:ILE:HG23	3:B:867:PRO:N	1.89	0.87
3:A:627:PHE:HE1	3:A:843:LEU:CA	1.87	0.87
3:A:1129:LYS:CA	3:A:1200:PRO:CA	2.42	0.87
3:B:743:TYR:CA	3:B:813:PHE:N	2.38	0.86
1:C:15:DG:N1	2:D:14:DA:C2	2.42	0.86
3:B:539:PHE:CZ	3:B:559:ILE:HG21	2.09	0.86
1:E:8:DT:H5''	3:B:622:LEU:HD21	1.57	0.86
1:E:14:DT:C4'	3:B:509:ARG:NH2	2.36	0.86
3:A:698:ARG:HG3	3:A:701:PRO:CG	2.05	0.86
1:E:8:DT:C5'	3:B:622:LEU:CD2	2.53	0.86
3:B:627:PHE:CE1	3:B:843:LEU:HA	2.10	0.86
1:C:8:DT:O3'	3:A:623:ARG:N	2.09	0.86
3:A:1028:THR:HG23	3:A:1030:GLU:HB3	1.58	0.86
3:B:492:ILE:CG1	3:B:580:VAL:CG2	2.26	0.86
1:C:10:DG:O4'	3:A:576:ALA:HA	1.76	0.86
1:C:9:DG:N3	3:A:576:ALA:HB2	1.91	0.86
1:C:15:DG:C2	2:D:14:DA:N3	2.43	0.86
3:A:1024:VAL:HG22	3:A:1200:PRO:HD2	1.56	0.86
1:E:8:DT:C3'	3:B:623:ARG:H	1.89	0.86
3:B:455:ASN:ND2	3:B:760:GLY:C	2.32	0.86
3:B:574:VAL:CG2	3:B:601:VAL:HG22	2.01	0.86
2:D:21:DOC:H3'1	5:A:1222:DTP:C5'	2.06	0.85
2:F:21:DOC:H4'	3:B:618:ASP:OD1	1.76	0.85
3:B:627:PHE:CA	3:B:846:VAL:HG21	2.06	0.85
3:B:831:VAL:HG11	3:B:839:PHE:HD1	1.38	0.85
3:A:455:ASN:ND2	3:A:760:GLY:C	2.32	0.85
3:A:774:VAL:CG2	3:B:778:GLN:HG2	2.06	0.85
3:A:743:TYR:C	3:A:813:PHE:N	2.34	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:994:ASP:CB	3:A:1017:ARG:NH2	2.39	0.85
3:B:458:ARG:HD2	3:B:764:LEU:HD21	1.58	0.85
1:C:11:DC:OP1	1:C:11:DC:H3'	1.75	0.85
1:C:8:DT:H3'	3:A:623:ARG:N	1.85	0.85
3:A:424:ARG:HH11	5:A:1222:DTP:H4'	1.33	0.85
3:A:858:ILE:CD1	3:A:889:PHE:CE1	2.60	0.85
3:A:1027:CYS:SG	3:A:1031:GLU:HB3	2.14	0.85
3:B:491:GLN:CG	3:B:574:VAL:HG11	2.07	0.85
3:B:548:GLU:O	3:B:550:GLU:N	2.10	0.85
3:A:627:PHE:CE1	3:A:843:LEU:CA	2.59	0.85
3:B:832:LYS:N	3:B:839:PHE:CE1	2.44	0.85
3:A:546:ARG:NH1	3:A:547:ALA:HB2	1.91	0.85
3:A:845:SER:HG	3:A:879:ASP:CG	1.82	0.85
3:B:448:LEU:HD22	3:B:816:SER:N	1.90	0.85
3:B:51:PHE:CE2	3:B:603:GLN:HG2	2.11	0.85
3:B:294:ARG:HB2	3:B:613:GLY:O	1.77	0.85
3:B:321:ARG:HH22	3:B:440:ASN:HD21	0.85	0.85
3:B:866:ILE:HG22	3:B:867:PRO:O	1.76	0.85
3:A:696:LEU:HD21	3:A:742:VAL:HG22	0.89	0.85
3:B:54:VAL:HG23	3:B:604:TYR:CE2	2.09	0.85
3:B:58:LYS:CB	3:B:287:ILE:HD12	2.06	0.85
3:B:539:PHE:HZ	3:B:559:ILE:HG23	1.42	0.85
2:D:20:DA:C2'	2:D:21:DOC:H5'	2.05	0.84
1:C:11:DC:H4'	3:A:573:SER:CB	2.07	0.84
1:E:6:DT:H2''	1:E:7:DG:OP2	1.77	0.84
3:A:575:HIS:HD2	3:A:577:ALA:C	1.85	0.84
3:B:744:GLN:HG3	3:B:813:PHE:HA	1.58	0.84
3:B:996:ILE:CD1	3:B:1017:ARG:HD2	1.74	0.84
1:E:9:DG:H1'	1:E:10:DG:H5''	1.59	0.84
3:A:855:ALA:CB	3:A:1008:ILE:HG21	1.67	0.84
1:E:9:DG:H4'	3:B:621:GLY:H	1.41	0.84
1:E:9:DG:H2''	1:E:10:DG:C5'	2.08	0.84
3:A:844:LEU:HB2	3:A:880:PHE:CD1	2.12	0.84
3:B:711:ARG:HD3	3:B:718:VAL:HG22	1.60	0.84
2:F:13:DC:H1'	2:F:14:DA:O5'	1.78	0.84
3:B:447:GLY:H	3:B:815:LYS:HZ2	0.84	0.84
1:C:9:DG:OP1	3:A:470:ASP:CB	2.26	0.84
3:A:539:PHE:HZ	3:A:559:ILE:HG23	1.42	0.83
3:A:743:TYR:CA	3:A:813:PHE:N	2.41	0.83
3:B:1123:GLU:O	3:B:1126:GLU:CD	2.21	0.83
3:B:699:PRO:C	3:B:701:PRO:CD	2.51	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:774:VAL:HG23	3:B:778:GLN:CG	2.07	0.83
3:A:774:VAL:HG21	3:B:778:GLN:HA	1.61	0.83
3:A:1118:VAL:CG1	3:A:1119:TRP:N	2.41	0.83
3:B:627:PHE:CB	3:B:846:VAL:HG21	2.09	0.83
3:A:1024:VAL:CG2	3:A:1200:PRO:CD	2.57	0.83
3:B:546:ARG:CD	3:B:546:ARG:C	2.51	0.83
3:B:832:LYS:CA	3:B:839:PHE:CD2	2.60	0.83
3:B:858:ILE:CD1	3:B:889:PHE:CZ	2.61	0.83
3:B:424:ARG:CZ	5:B:1222:DTP:C4'	2.56	0.83
3:A:523:LYS:HD2	3:A:1094:LYS:HZ2	1.42	0.83
1:C:16:DG:O6	2:D:12:DC:N3	2.12	0.82
3:A:671:GLU:OE2	3:A:853:LYS:NZ	2.12	0.82
3:B:858:ILE:HD11	3:B:889:PHE:CZ	2.14	0.82
3:B:1035:PHE:HA	3:B:1170:GLY:CA	2.09	0.82
3:A:862:ARG:NE	3:A:868:VAL:HB	1.93	0.82
3:A:1046:LEU:HD21	3:A:1202:ARG:NE	1.94	0.82
1:C:14:DT:H4'	3:A:509:ARG:HH12	1.44	0.82
3:A:492:ILE:CD1	3:A:616:LYS:CG	2.58	0.82
3:A:627:PHE:CB	3:A:846:VAL:HG21	2.09	0.82
1:C:9:DG:C5'	3:A:621:GLY:N	2.43	0.82
3:A:425:GLY:H	3:A:817:HIS:CD2	1.96	0.82
3:B:743:TYR:HA	3:B:813:PHE:N	1.94	0.82
2:F:14:DA:H1'	2:F:15:DG:C8	2.15	0.82
3:A:546:ARG:CD	3:A:546:ARG:C	2.52	0.82
3:A:858:ILE:HD13	3:A:889:PHE:CZ	2.10	0.82
3:B:424:ARG:CZ	5:B:1222:DTP:H4'	2.10	0.82
3:B:665:LYS:HD3	3:B:860:ASP:CG	2.04	0.82
1:E:9:DG:H2''	1:E:10:DG:H5'	1.61	0.82
3:B:627:PHE:HB2	3:B:846:VAL:HG11	1.61	0.82
3:B:832:LYS:CA	3:B:839:PHE:CE2	2.63	0.82
3:A:521:LEU:HD21	3:A:548:GLU:HG2	1.61	0.81
3:A:696:LEU:CG	3:A:742:VAL:HG13	2.09	0.81
3:A:776:GLU:HG3	3:B:774:VAL:HG12	1.59	0.81
3:A:745:GLU:CD	3:A:814:ASN:HA	2.06	0.81
3:A:1028:THR:CG2	3:A:1030:GLU:HB3	2.10	0.81
3:B:535:LEU:HD23	3:B:539:PHE:CE1	2.16	0.81
1:C:8:DT:OP1	3:A:623:ARG:CB	2.28	0.81
1:C:9:DG:N3	3:A:576:ALA:HB3	1.93	0.81
2:D:18:DC:H2''	2:D:19:DC:OP2	1.79	0.81
3:A:234:THR:O	3:A:510:VAL:CG1	2.29	0.81
3:A:424:ARG:CZ	5:A:1222:DTP:O3'	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:535:LEU:HD23	3:A:539:PHE:CE1	2.16	0.81
3:B:458:ARG:CZ	3:B:764:LEU:CD1	2.58	0.81
1:E:17:DC:H2''	1:E:18:DC:OP2	1.80	0.81
2:F:12:DC:H2''	2:F:13:DC:OP2	1.78	0.81
3:A:546:ARG:C	3:A:546:ARG:HD3	2.05	0.81
3:B:665:LYS:CD	3:B:860:ASP:CG	2.50	0.81
2:D:19:DC:OP2	3:A:531:LYS:HE2	1.79	0.81
3:A:575:HIS:HD2	3:A:578:GLY:CA	1.92	0.81
1:C:8:DT:P	3:A:623:ARG:CB	2.65	0.81
3:B:424:ARG:CZ	5:B:1222:DTP:O4'	2.29	0.81
3:B:696:LEU:HD21	3:B:742:VAL:HG22	0.84	0.81
2:D:19:DC:H2'	3:A:531:LYS:HZ2	1.42	0.81
1:C:14:DT:O4	2:D:14:DA:N6	2.14	0.80
1:C:15:DG:N2	2:D:14:DA:N3	2.29	0.80
3:A:492:ILE:HG21	3:A:606:MET:HA	1.61	0.80
3:B:452:ARG:HG3	3:B:748:MET:SD	2.21	0.80
3:B:714:GLY:O	3:B:715:GLN:CG	2.29	0.80
3:B:858:ILE:CD1	3:B:889:PHE:HZ	1.94	0.80
1:C:9:DG:H4'	3:A:621:GLY:H	0.65	0.80
3:A:455:ASN:CG	3:A:760:GLY:CA	2.53	0.80
3:A:1028:THR:HG22	3:A:1031:GLU:HG3	1.64	0.80
1:C:9:DG:OP1	3:A:470:ASP:HB2	1.82	0.80
3:A:575:HIS:CG	3:A:578:GLY:N	2.40	0.80
3:A:744:GLN:H	3:A:813:PHE:CA	1.95	0.80
3:A:1013:HIS:ND1	3:A:1073:GLU:HB2	1.95	0.80
3:A:866:ILE:HG22	3:A:867:PRO:N	1.96	0.80
3:B:627:PHE:HE1	3:B:842:ALA:C	1.90	0.80
3:B:1125:LEU:O	3:B:1126:GLU:CG	2.30	0.80
3:A:1034:GLU:CD	3:A:1170:GLY:HA2	2.07	0.80
3:B:866:ILE:HG23	3:B:867:PRO:CD	2.11	0.80
3:B:743:TYR:H	3:B:746:GLN:HE21	1.30	0.79
3:B:844:LEU:CB	3:B:880:PHE:CD1	2.59	0.79
2:F:20:DA:H2''	2:F:21:DOC:C5'	2.10	0.79
3:A:743:TYR:H	3:A:746:GLN:HE21	1.30	0.79
3:A:774:VAL:CG2	3:B:778:GLN:CG	2.60	0.79
3:A:775:GLU:CD	3:B:781:ARG:HH21	1.90	0.79
3:B:744:GLN:N	3:B:813:PHE:C	2.36	0.79
1:E:8:DT:H5''	3:B:622:LEU:HD23	1.62	0.79
2:F:14:DA:H2''	2:F:15:DG:OP2	1.82	0.79
3:A:458:ARG:HD2	3:A:764:LEU:HD21	1.62	0.79
3:A:575:HIS:CB	3:A:578:GLY:HA3	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:LYS:NZ	3:A:1054:VAL:HG22	1.97	0.79
3:A:665:LYS:HD3	3:A:860:ASP:CG	2.08	0.79
3:A:776:GLU:CB	3:B:775:GLU:HG3	2.12	0.79
3:A:999:LEU:HD11	3:A:1013:HIS:H	1.46	0.79
3:B:1140:LEU:HD12	3:B:1143:LYS:HZ1	1.44	0.79
2:F:9:DC:H2''	2:F:10:DG:OP2	1.82	0.79
3:B:701:PRO:HD3	3:B:811:TYR:CG	2.18	0.79
3:B:1035:PHE:HD1	3:B:1171:GLU:N	1.76	0.79
1:C:9:DG:C4'	3:A:621:GLY:CA	2.60	0.79
3:A:566:GLU:O	3:A:568:LEU:N	2.16	0.79
3:B:492:ILE:HG13	3:B:580:VAL:HG22	0.79	0.78
1:C:10:DG:O4'	3:A:576:ALA:CB	2.30	0.78
3:B:546:ARG:CD	3:B:547:ALA:N	2.44	0.78
3:B:1026:SER:OG	3:B:1046:LEU:O	2.01	0.78
3:B:704:HIS:NE2	3:B:808:PHE:HZ	1.80	0.78
2:D:13:DC:H2''	2:D:14:DA:OP2	1.82	0.78
3:A:424:ARG:NE	5:A:1222:DTP:O3'	2.17	0.78
3:A:455:ASN:CG	3:A:760:GLY:HA3	2.08	0.78
3:A:845:SER:OG	3:A:879:ASP:CG	2.26	0.78
3:B:8:ALA:H	3:B:274:THR:HG21	1.49	0.78
3:A:523:LYS:HD2	3:A:1094:LYS:HZ1	1.44	0.78
3:B:455:ASN:OD1	3:B:760:GLY:HA3	1.83	0.78
3:B:999:LEU:CB	3:B:1014:PRO:CG	2.61	0.78
3:A:1118:VAL:HG13	3:A:1119:TRP:H	1.49	0.78
3:B:424:ARG:CD	5:B:1222:DTP:H4'	2.14	0.78
1:C:23:DT:H1'	1:C:24:DT:O5'	1.82	0.78
2:D:19:DC:P	3:A:531:LYS:NZ	2.57	0.78
3:B:574:VAL:CG2	3:B:601:VAL:HG21	2.09	0.78
3:A:8:ALA:H	3:A:274:THR:HG21	1.49	0.78
3:B:1046:LEU:HD21	3:B:1202:ARG:HH21	0.65	0.77
3:A:230:ILE:HD12	3:A:565:LEU:CD1	2.14	0.77
3:A:574:VAL:HG23	3:A:601:VAL:HG21	1.66	0.77
3:A:697:TYR:CZ	3:A:702:MET:HE1	2.18	0.77
3:A:844:LEU:CG	3:A:880:PHE:CE1	2.68	0.77
3:B:567:GLY:C	3:B:568:LEU:N	2.42	0.77
3:B:832:LYS:HE3	3:B:840:MET:HE1	1.67	0.77
2:F:18:DC:H2''	2:F:19:DC:OP2	1.83	0.77
3:B:51:PHE:HE2	3:B:603:GLN:HG2	1.49	0.77
2:D:14:DA:H2''	2:D:15:DG:OP2	1.83	0.77
3:A:845:SER:CA	3:A:879:ASP:OD1	2.28	0.77
3:A:627:PHE:HA	3:A:846:VAL:CG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:DOC:H2''	3:A:424:ARG:HH12	0.96	0.77
3:A:230:ILE:HD13	3:A:565:LEU:CD1	1.97	0.77
3:A:699:PRO:O	3:A:811:TYR:CE2	2.37	0.77
3:A:634:ILE:HG21	3:A:838:GLU:CB	2.10	0.76
3:A:1099:LEU:CD2	3:A:1119:TRP:O	2.33	0.76
3:A:745:GLU:OE1	3:A:814:ASN:HA	1.86	0.76
3:B:491:GLN:C	3:B:492:ILE:C	2.53	0.76
1:C:13:DC:H1'	1:C:14:DT:H5''	1.65	0.76
1:C:16:DG:N1	2:D:13:DC:O2	2.18	0.76
3:A:866:ILE:CG2	3:A:867:PRO:N	2.48	0.76
3:B:455:ASN:ND2	3:B:760:GLY:HA2	1.99	0.76
3:B:999:LEU:CB	3:B:1014:PRO:HG3	2.15	0.76
1:C:8:DT:OP2	3:A:623:ARG:CB	2.33	0.76
2:F:21:DOC:H2''	3:B:424:ARG:HH11	0.88	0.76
3:A:865:GLY:O	3:A:866:ILE:CG1	2.33	0.76
3:B:844:LEU:HB3	3:B:880:PHE:CE1	2.21	0.76
3:B:866:ILE:HG23	3:B:867:PRO:HD2	1.68	0.76
1:E:18:DC:OP1	3:B:933:ARG:HD3	1.86	0.76
1:E:17:DC:H5''	3:B:933:ARG:NH2	2.01	0.76
3:B:627:PHE:HA	3:B:846:VAL:CG2	2.15	0.76
3:A:858:ILE:HD11	3:A:889:PHE:CE1	2.16	0.75
3:A:994:ASP:HB2	3:A:1017:ARG:NH1	2.01	0.75
1:C:15:DG:C2	1:C:16:DG:C5	2.74	0.75
3:A:697:TYR:OH	3:A:702:MET:HE1	1.86	0.75
3:A:698:ARG:CG	3:A:701:PRO:CG	2.64	0.75
3:A:699:PRO:C	3:A:701:PRO:CD	2.57	0.75
3:A:862:ARG:HH22	3:A:1010:VAL:HG13	1.51	0.75
3:A:546:ARG:NH2	3:A:547:ALA:HB2	2.01	0.75
3:B:667:VAL:HA	3:B:828:THR:HG21	1.69	0.75
3:B:698:ARG:O	3:B:701:PRO:HD2	1.86	0.75
1:E:15:DG:H1'	1:E:16:DG:H5'	1.67	0.75
3:A:696:LEU:HD11	3:A:742:VAL:HG21	1.67	0.75
3:B:491:GLN:C	3:B:492:ILE:O	2.29	0.75
1:C:10:DG:O4'	3:A:576:ALA:CA	2.34	0.75
3:A:667:VAL:HA	3:A:828:THR:HG21	1.69	0.75
1:C:9:DG:N3	3:A:576:ALA:HB1	2.01	0.75
2:F:21:DOC:H6	2:F:21:DOC:H5''	1.69	0.75
3:A:574:VAL:CB	3:A:601:VAL:HG22	2.15	0.75
2:D:21:DOC:C2'	5:A:1222:DTP:C4'	2.64	0.75
1:E:10:DG:C4'	3:B:576:ALA:CB	2.65	0.74
3:A:539:PHE:CE2	3:A:559:ILE:HG21	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:627:PHE:HE1	3:B:843:LEU:CA	2.00	0.74
1:C:15:DG:C6	2:D:14:DA:N1	2.55	0.74
2:D:12:DC:H2''	2:D:13:DC:C6	2.22	0.74
3:A:547:ALA:O	3:A:549:MET:N	2.19	0.74
3:A:858:ILE:HD13	3:A:889:PHE:CE1	2.22	0.74
2:F:4:DA:H2''	2:F:5:DA:OP2	1.86	0.74
3:A:745:GLU:OE2	3:A:814:ASN:HA	1.85	0.74
3:A:844:LEU:HD13	3:A:880:PHE:CD2	2.21	0.74
3:A:1013:HIS:HD2	3:A:1015:VAL:N	1.82	0.74
3:B:710:ARG:NH1	3:B:716:GLU:CD	2.45	0.74
3:A:230:ILE:HD12	3:A:565:LEU:HD11	1.69	0.74
3:B:539:PHE:CE2	3:B:559:ILE:HG21	2.22	0.74
3:B:1140:LEU:HB2	3:B:1143:LYS:HD2	1.70	0.74
1:C:14:DT:O2	2:D:15:DG:C2	2.40	0.74
1:C:9:DG:H3'	1:C:9:DG:OP1	1.88	0.74
1:E:9:DG:C2'	1:E:10:DG:C5'	2.66	0.74
3:B:1126:GLU:HG3	3:B:1205:PHE:HE2	1.50	0.74
2:F:21:DOC:C2'	3:B:424:ARG:HH11	1.84	0.74
3:A:698:ARG:CG	3:A:701:PRO:HG2	2.18	0.74
2:D:14:DA:OP1	2:D:14:DA:H3'	1.88	0.74
3:A:774:VAL:CG2	3:B:778:GLN:CA	2.65	0.74
3:B:994:ASP:OD2	3:B:1017:ARG:CZ	2.35	0.74
3:B:627:PHE:CE1	3:B:843:LEU:CA	2.70	0.74
1:E:10:DG:O4'	3:B:576:ALA:CB	2.35	0.73
3:A:1028:THR:O	3:A:1030:GLU:N	2.20	0.73
3:B:425:GLY:H	3:B:817:HIS:CD2	2.06	0.73
3:B:665:LYS:HD2	3:B:860:ASP:HB3	1.70	0.73
3:A:845:SER:HA	3:A:879:ASP:CG	2.12	0.73
3:A:1013:HIS:N	3:A:1014:PRO:HD3	1.70	0.73
2:D:9:DC:C1'	2:D:10:DG:H5''	2.13	0.73
3:A:538:ALA:O	3:A:539:PHE:CD1	2.42	0.73
3:A:776:GLU:OE1	3:B:775:GLU:OE2	2.06	0.73
3:B:538:ALA:O	3:B:539:PHE:CD1	2.42	0.73
1:E:17:DC:H3'	3:B:933:ARG:NH1	2.02	0.73
3:A:294:ARG:HB2	3:A:614:LEU:HD23	1.70	0.73
3:A:779:LYS:HZ2	3:B:774:VAL:CA	2.01	0.73
3:B:58:LYS:HB3	3:B:287:ILE:HD12	1.67	0.73
3:B:660:SER:HB3	3:B:683:LYS:HD3	1.71	0.73
3:B:817:HIS:CE1	5:B:1222:DTP:C2'	2.69	0.73
3:A:1046:LEU:CD2	3:A:1202:ARG:HE	2.02	0.73
3:B:448:LEU:HD13	3:B:816:SER:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:844:LEU:HB3	3:B:880:PHE:HD1	1.51	0.73
2:F:19:DC:H5''	3:B:531:LYS:HZ3	1.54	0.73
3:A:523:LYS:CD	3:A:1054:VAL:HG13	2.17	0.73
3:A:660:SER:HB3	3:A:683:LYS:HD3	1.71	0.73
3:A:845:SER:CB	3:A:879:ASP:CG	2.62	0.73
3:B:744:GLN:HG3	3:B:813:PHE:CA	2.19	0.73
1:C:16:DG:O6	2:D:12:DC:C2	2.42	0.73
3:A:8:ALA:H	3:A:274:THR:CG2	2.01	0.73
3:B:996:ILE:HD11	3:B:1017:ARG:HD3	1.67	0.73
3:A:1035:PHE:HD1	3:A:1171:GLU:O	1.70	0.72
3:A:858:ILE:HD12	3:A:1008:ILE:CD1	2.18	0.72
3:B:832:LYS:HA	3:B:839:PHE:CG	2.24	0.72
3:B:996:ILE:CG1	3:B:1017:ARG:HB2	2.14	0.72
1:C:9:DG:H3'	3:A:621:GLY:CA	2.14	0.72
3:A:547:ALA:O	3:A:550:GLU:N	2.22	0.72
3:B:8:ALA:H	3:B:274:THR:CG2	2.01	0.72
3:A:407:GLN:HG3	3:A:436:VAL:HG12	1.72	0.72
3:A:1024:VAL:HG21	3:A:1200:PRO:HG2	1.70	0.72
3:A:1118:VAL:HG12	3:A:1119:TRP:N	2.03	0.72
1:C:9:DG:P	1:C:9:DG:H2'	2.28	0.72
3:A:37:PRO:HB2	3:B:459:VAL:HG21	1.71	0.72
3:A:832:LYS:HB2	3:A:839:PHE:HE2	1.51	0.72
1:C:11:DC:H3'	1:C:11:DC:P	2.30	0.72
3:B:1035:PHE:HB2	3:B:1170:GLY:HA2	1.71	0.72
1:E:23:DT:H2''	1:E:24:DT:OP2	1.88	0.72
3:A:774:VAL:HG21	3:B:778:GLN:CA	2.20	0.72
3:B:832:LYS:N	3:B:839:PHE:CD1	2.58	0.72
1:C:9:DG:C3'	3:A:621:GLY:CA	2.67	0.72
3:A:696:LEU:HG	3:A:742:VAL:HG11	1.71	0.72
3:B:491:GLN:CD	3:B:574:VAL:HG11	2.14	0.72
1:C:9:DG:OP1	3:A:470:ASP:HB3	1.90	0.72
1:C:23:DT:H2''	1:C:24:DT:OP2	1.87	0.72
3:A:523:LYS:HD3	3:A:1094:LYS:HZ3	1.50	0.72
3:B:407:GLN:HG3	3:B:436:VAL:HG12	1.72	0.72
3:A:1026:SER:OG	3:A:1046:LEU:O	2.07	0.71
1:C:16:DG:C6	2:D:13:DC:O2	2.43	0.71
3:B:446:PHE:HB3	3:B:815:LYS:HE2	1.71	0.71
3:B:448:LEU:CD1	3:B:816:SER:HA	2.21	0.71
1:C:8:DT:C4'	3:A:623:ARG:H	2.03	0.71
3:A:257:MET:HE2	3:A:257:MET:HA	1.72	0.71
3:A:627:PHE:HB2	3:A:846:VAL:HG21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:996:ILE:HD13	3:B:1018:TYR:CE2	2.25	0.71
3:B:996:ILE:HD12	3:B:1017:ARG:HD3	0.73	0.71
3:A:776:GLU:HG3	3:B:775:GLU:CG	2.18	0.71
3:B:458:ARG:CZ	3:B:764:LEU:CD2	2.69	0.71
3:B:701:PRO:CD	3:B:811:TYR:CD1	2.72	0.71
1:C:10:DG:H1'	1:C:11:DC:C5'	2.20	0.71
2:F:19:DC:P	3:B:531:LYS:HE2	2.30	0.71
3:A:491:GLN:C	3:A:492:ILE:N	2.48	0.71
3:B:257:MET:HA	3:B:257:MET:HE2	1.72	0.71
3:B:458:ARG:CZ	3:B:764:LEU:HD13	2.20	0.71
3:B:832:LYS:CB	3:B:839:PHE:CD2	2.73	0.71
2:D:9:DC:H2''	2:D:10:DG:OP2	1.90	0.71
1:E:17:DC:H3'	3:B:933:ARG:CZ	2.20	0.71
1:E:20:DT:H2''	1:E:21:DC:OP2	1.89	0.71
3:B:745:GLU:OE2	3:B:814:ASN:ND2	2.24	0.71
3:B:699:PRO:O	3:B:701:PRO:HD2	1.90	0.71
3:A:696:LEU:HD21	3:A:742:VAL:CB	2.21	0.70
1:E:9:DG:H1'	1:E:10:DG:H5'	1.71	0.70
3:A:776:GLU:CB	3:B:775:GLU:CG	2.69	0.70
3:A:1159:LEU:HD11	3:A:1183:GLU:HG2	1.72	0.70
3:B:492:ILE:HA	3:B:602:THR:OG1	1.91	0.70
3:B:537:GLU:O	3:B:539:PHE:N	2.24	0.70
3:B:575:HIS:CB	3:B:578:GLY:HA3	2.03	0.70
1:E:9:DG:H4'	3:B:621:GLY:N	2.06	0.70
2:F:13:DC:H2''	2:F:14:DA:OP2	1.90	0.70
3:A:858:ILE:HD12	3:A:1008:ILE:HD13	1.72	0.70
3:B:996:ILE:CD1	3:B:1017:ARG:CB	2.65	0.70
3:A:1118:VAL:CG1	3:A:1119:TRP:H	2.00	0.70
3:B:996:ILE:HD13	3:B:1018:TYR:HE2	1.56	0.70
2:F:21:DOC:C4'	3:B:618:ASP:OD1	2.39	0.70
3:A:776:GLU:OE1	3:B:775:GLU:CD	2.34	0.70
3:B:546:ARG:NH2	3:B:547:ALA:HB2	2.03	0.70
1:E:18:DC:OP1	3:B:933:ARG:CB	2.31	0.70
3:A:696:LEU:O	3:A:701:PRO:HB2	1.91	0.70
3:B:58:LYS:NZ	3:B:608:ALA:HA	2.06	0.70
3:B:110:VAL:CG1	3:B:587:THR:O	2.40	0.70
3:A:496:GLY:O	3:A:569:ASN:HB3	1.92	0.70
3:A:1129:LYS:O	3:A:1130:ALA:HB2	1.92	0.70
3:B:704:HIS:CE1	3:B:808:PHE:HZ	2.10	0.70
2:D:13:DC:H1'	2:D:14:DA:O5'	1.92	0.69
3:A:835:TYR:O	3:A:839:PHE:HB3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:844:LEU:CD2	3:B:880:PHE:CE1	2.72	0.69
3:A:779:LYS:HZ1	3:B:774:VAL:HA	1.57	0.69
3:B:58:LYS:HB2	3:B:287:ILE:HD13	1.72	0.69
3:B:1159:LEU:HD11	3:B:1183:GLU:HG2	1.72	0.69
2:D:12:DC:H3'	2:D:12:DC:OP1	1.92	0.69
1:E:17:DC:O3'	3:B:933:ARG:CD	2.40	0.69
3:A:774:VAL:CG2	3:B:778:GLN:HA	2.21	0.69
3:A:994:ASP:HB3	3:A:1017:ARG:HH22	1.56	0.69
3:A:1129:LYS:O	3:A:1130:ALA:CB	2.40	0.69
3:B:491:GLN:C	3:B:492:ILE:CA	2.64	0.69
1:C:8:DT:H5''	3:A:622:LEU:HD23	0.70	0.69
3:A:537:GLU:O	3:A:539:PHE:N	2.24	0.69
3:B:547:ALA:O	3:B:550:GLU:HB2	1.91	0.69
3:B:1176:LEU:HD23	3:B:1179:VAL:HB	1.75	0.69
1:C:10:DG:H1'	1:C:11:DC:H5'	1.72	0.69
3:A:665:LYS:CD	3:A:860:ASP:CG	2.66	0.69
1:C:8:DT:H3'	3:A:623:ARG:HB2	1.75	0.69
3:A:492:ILE:HG13	3:A:580:VAL:CG2	2.20	0.69
3:A:634:ILE:CG2	3:A:838:GLU:HB2	2.22	0.69
3:A:698:ARG:HG2	3:A:701:PRO:HG2	1.73	0.69
3:A:699:PRO:C	3:A:811:TYR:CD2	2.70	0.69
3:B:58:LYS:HB3	3:B:287:ILE:HD11	1.74	0.69
3:B:845:SER:HA	3:B:879:ASP:CG	2.18	0.69
3:A:458:ARG:NH2	3:A:764:LEU:CD1	2.56	0.69
3:A:523:LYS:HZ1	3:A:1054:VAL:HG22	1.57	0.69
3:A:699:PRO:O	3:A:701:PRO:CD	2.41	0.69
3:B:54:VAL:CG2	3:B:604:TYR:CD1	2.69	0.68
3:B:696:LEU:CG	3:B:742:VAL:HG22	2.23	0.68
3:B:58:LYS:HB2	3:B:287:ILE:HD12	1.72	0.68
3:B:866:ILE:HG22	3:B:867:PRO:CA	2.22	0.68
3:A:458:ARG:NH2	3:A:764:LEU:HD22	2.08	0.68
3:A:994:ASP:HB3	3:A:1017:ARG:NH2	2.08	0.68
3:B:832:LYS:CB	3:B:839:PHE:CZ	2.57	0.68
3:B:744:GLN:N	3:B:813:PHE:CA	2.52	0.68
2:F:7:DG:H2''	2:F:8:DA:OP2	1.94	0.68
3:A:575:HIS:CD2	3:A:577:ALA:C	2.67	0.68
3:B:831:VAL:CG1	3:B:839:PHE:CE1	2.69	0.68
2:D:14:DA:H1'	2:D:15:DG:C8	2.29	0.68
3:A:745:GLU:CD	3:A:815:LYS:H	2.02	0.68
3:B:627:PHE:CE1	3:B:842:ALA:C	2.72	0.68
3:A:457:GLU:OE2	3:A:758:SER:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:665:LYS:HZ3	3:A:864:LEU:HD13	1.57	0.68
3:A:1176:LEU:HD23	3:A:1179:VAL:HB	1.75	0.68
3:B:1013:HIS:HB3	3:B:1015:VAL:HG12	1.76	0.68
3:B:701:PRO:CD	3:B:811:TYR:CG	2.77	0.67
2:D:19:DC:OP2	3:A:531:LYS:CE	2.41	0.67
2:D:19:DC:H5''	3:A:531:LYS:NZ	2.09	0.67
2:F:5:DA:H2''	2:F:6:DC:OP2	1.93	0.67
3:B:602:THR:HG22	3:B:604:TYR:H	1.60	0.67
3:B:699:PRO:HB2	3:B:811:TYR:OH	1.94	0.67
1:C:22:DG:C4	2:D:7:DG:N2	2.62	0.67
1:C:9:DG:C2	3:A:576:ALA:CB	2.77	0.67
3:A:665:LYS:HD3	3:A:860:ASP:CB	2.25	0.67
3:A:699:PRO:C	3:A:701:PRO:HD2	2.17	0.67
3:A:1120:THR:O	3:A:1124:VAL:CG2	2.35	0.67
3:B:627:PHE:CE1	3:B:843:LEU:N	2.54	0.67
3:B:1021:LEU:HD23	3:B:1124:VAL:HG11	1.76	0.67
3:A:1028:THR:O	3:A:1029:ILE:C	2.37	0.67
3:B:1035:PHE:HE1	3:B:1171:GLU:C	1.97	0.67
3:A:638:SER:OG	3:A:838:GLU:OE1	2.11	0.67
1:E:15:DG:C2	2:F:14:DA:C2	2.83	0.67
3:B:546:ARG:HD3	3:B:547:ALA:H	1.59	0.67
3:B:1125:LEU:O	3:B:1126:GLU:CB	2.42	0.67
3:A:773:ARG:NH1	3:B:775:GLU:OE1	2.28	0.67
3:B:832:LYS:CG	3:B:839:PHE:CE2	2.78	0.67
1:E:10:DG:H5''	3:B:576:ALA:HB1	1.76	0.67
1:E:15:DG:H1'	1:E:16:DG:C5'	2.25	0.67
3:A:832:LYS:HA	3:A:839:PHE:CD2	2.29	0.67
3:A:698:ARG:HG3	3:A:701:PRO:CD	2.24	0.66
1:C:8:DT:H5'	3:A:622:LEU:HD21	1.75	0.66
3:A:77:ALA:O	3:A:129:ARG:NH2	2.28	0.66
3:A:776:GLU:CG	3:B:775:GLU:CG	2.73	0.66
1:C:10:DG:O4'	3:A:576:ALA:HB2	1.93	0.66
3:B:627:PHE:CZ	3:B:843:LEU:HG	2.30	0.66
3:B:999:LEU:HD22	3:B:1012:GLY:O	1.95	0.66
1:E:8:DT:C1'	1:E:9:DG:O5'	2.37	0.66
3:B:452:ARG:HH21	3:B:766:ARG:NE	1.93	0.66
3:B:538:ALA:C	3:B:539:PHE:CD1	2.74	0.66
3:B:743:TYR:HA	3:B:813:PHE:CA	2.26	0.66
3:B:831:VAL:C	3:B:839:PHE:CD1	2.73	0.66
3:A:535:LEU:CD2	3:A:539:PHE:CE1	2.78	0.66
1:E:10:DG:H4'	3:B:576:ALA:CA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1019:PRO:O	3:A:1023:GLU:HG2	1.96	0.66
3:B:996:ILE:CD1	3:B:1018:TYR:CE2	2.79	0.66
1:C:13:DC:H2''	1:C:14:DT:H5'	1.77	0.66
2:D:21:DOC:C3'	5:A:1222:DTP:H5'1	2.20	0.66
1:E:9:DG:C2'	1:E:10:DG:H5'	2.24	0.66
3:B:1019:PRO:O	3:B:1023:GLU:HG2	1.96	0.66
1:C:10:DG:H5'	3:A:576:ALA:O	1.96	0.66
3:A:425:GLY:H	3:A:817:HIS:HD2	1.40	0.66
2:D:5:DA:H1'	2:D:6:DC:O5'	1.95	0.66
3:A:538:ALA:C	3:A:539:PHE:CD1	2.74	0.66
3:B:744:GLN:OE1	3:B:814:ASN:HB2	1.96	0.66
3:B:951:ALA:HB2	3:B:993:LEU:HG	1.78	0.66
3:A:285:LEU:HB3	3:A:286:PRO:CD	2.26	0.66
3:A:696:LEU:CG	3:A:742:VAL:CG1	2.70	0.66
3:B:996:ILE:CG1	3:B:1017:ARG:HB3	2.17	0.66
1:C:15:DG:C4	1:C:16:DG:N7	2.64	0.65
1:E:8:DT:H2''	1:E:9:DG:OP2	1.96	0.65
3:B:77:ALA:O	3:B:129:ARG:NH2	2.28	0.65
3:B:698:ARG:O	3:B:701:PRO:HG2	1.96	0.65
1:C:14:DT:O3'	3:A:509:ARG:CZ	2.43	0.65
1:E:9:DG:C1'	1:E:10:DG:C5'	2.73	0.65
3:A:665:LYS:CG	3:A:860:ASP:OD2	2.44	0.65
3:B:448:LEU:HD13	3:B:816:SER:CB	2.26	0.65
3:B:535:LEU:CD2	3:B:539:PHE:CE1	2.78	0.65
3:B:999:LEU:HD21	3:B:1012:GLY:C	2.21	0.65
3:B:1152:LEU:HB3	3:B:1179:VAL:HG11	1.78	0.65
3:A:602:THR:HG22	3:A:604:TYR:H	1.60	0.65
2:F:21:DOC:C5'	2:F:21:DOC:H6	2.26	0.65
3:A:696:LEU:CD2	3:A:742:VAL:CG1	2.75	0.65
1:C:9:DG:H1'	3:A:576:ALA:HB1	1.78	0.65
1:E:8:DT:H3'	3:B:623:ARG:HB2	1.79	0.65
2:F:3:DA:H2''	2:F:4:DA:OP2	1.97	0.65
3:A:627:PHE:HE1	3:A:842:ALA:C	2.04	0.65
3:A:634:ILE:HG22	3:A:838:GLU:HB2	1.78	0.65
3:A:855:ALA:HB2	3:A:1008:ILE:HG22	0.80	0.65
1:C:15:DG:H2''	1:C:16:DG:OP2	1.96	0.65
2:D:12:DC:C2'	2:D:13:DC:C6	2.80	0.65
3:A:951:ALA:HB2	3:A:993:LEU:HG	1.78	0.65
3:A:546:ARG:HD3	3:A:547:ALA:N	2.12	0.65
3:A:774:VAL:N	3:B:778:GLN:HG2	2.06	0.65
1:C:17:DC:H2''	1:C:18:DC:OP2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:773:ARG:O	3:B:778:GLN:NE2	2.29	0.65
3:A:999:LEU:HD11	3:A:1013:HIS:N	2.04	0.65
3:B:835:TYR:O	3:B:839:PHE:HB2	1.97	0.65
3:B:1142:GLU:O	3:B:1143:LYS:HG3	1.96	0.65
3:B:828:THR:O	3:B:839:PHE:CZ	2.50	0.65
3:B:548:GLU:O	3:B:549:MET:C	2.40	0.64
3:B:700:GLY:HA3	3:B:811:TYR:CE1	2.32	0.64
3:B:858:ILE:HD13	3:B:889:PHE:HZ	1.62	0.64
1:E:8:DT:H4'	3:B:622:LEU:HA	1.78	0.64
3:A:455:ASN:CG	3:A:760:GLY:HA2	2.20	0.64
1:C:8:DT:H3'	3:A:623:ARG:CB	2.28	0.64
1:C:24:DT:C2'	1:C:25:DT:P	2.85	0.64
3:B:666:GLY:HA3	3:B:843:LEU:HD13	1.80	0.64
1:C:8:DT:C5'	3:A:622:LEU:HD21	2.18	0.64
1:C:12:DA:H2''	1:C:13:DC:OP2	1.96	0.64
3:A:697:TYR:HE1	3:A:702:MET:SD	2.13	0.64
3:A:775:GLU:CD	3:B:781:ARG:NH2	2.55	0.64
3:A:835:TYR:O	3:A:839:PHE:CB	2.46	0.64
3:B:458:ARG:NE	3:B:764:LEU:HD11	2.12	0.64
1:C:7:DG:H1'	1:C:8:DT:O5'	1.97	0.64
1:C:14:DT:C4'	3:A:509:ARG:HH12	2.11	0.64
1:E:9:DG:C1'	1:E:10:DG:H5''	2.26	0.64
3:A:458:ARG:HH12	3:A:764:LEU:HD22	1.51	0.64
3:A:1053:GLU:HB3	3:A:1068:PHE:HA	1.80	0.64
3:A:448:LEU:HD22	3:A:816:SER:HA	1.80	0.64
3:A:1028:THR:O	3:A:1028:THR:CG2	2.45	0.64
3:B:1023:GLU:O	3:B:1164:ARG:NH2	2.28	0.64
2:F:19:DC:OP2	2:F:19:DC:C6	2.51	0.64
3:A:697:TYR:CZ	3:A:702:MET:CE	2.80	0.64
3:B:858:ILE:HD13	3:B:889:PHE:CZ	2.31	0.64
3:B:1053:GLU:HB3	3:B:1068:PHE:HA	1.80	0.63
2:D:19:DC:H6	3:A:531:LYS:CE	2.11	0.63
1:E:8:DT:H1'	1:E:9:DG:C5'	2.28	0.63
3:B:698:ARG:O	3:B:701:PRO:CD	2.45	0.63
3:B:812:GLY:C	3:B:813:PHE:N	2.56	0.63
3:B:1035:PHE:CZ	3:B:1171:GLU:O	2.50	0.63
1:C:10:DG:H2''	1:C:11:DC:O5'	1.96	0.63
1:E:9:DG:C2	2:F:20:DA:N1	2.67	0.63
3:A:575:HIS:CB	3:A:578:GLY:H	2.12	0.63
3:A:1013:HIS:CD2	3:A:1015:VAL:CG1	2.81	0.63
1:C:15:DG:O6	2:D:13:DC:N3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:627:PHE:CE1	3:A:842:ALA:C	2.76	0.63
3:B:1140:LEU:HB2	3:B:1143:LYS:HZ2	1.63	0.63
3:B:455:ASN:CG	3:B:760:GLY:CA	2.70	0.63
3:B:714:GLY:C	3:B:715:GLN:HG3	2.24	0.63
3:A:665:LYS:HB2	3:A:832:LYS:HZ1	1.63	0.63
2:D:19:DC:OP2	2:D:19:DC:C6	2.51	0.63
1:E:11:DC:H4'	3:B:573:SER:OG	1.99	0.63
3:A:695:SER:HG	3:A:743:TYR:HE2	1.46	0.63
3:A:775:GLU:OE2	3:B:806:GLU:OE1	2.16	0.63
3:A:547:ALA:C	3:A:549:MET:N	2.52	0.63
3:A:665:LYS:CG	3:A:860:ASP:CG	2.72	0.63
3:A:699:PRO:C	3:A:811:TYR:CE2	2.77	0.63
3:B:458:ARG:CZ	3:B:764:LEU:HD11	2.28	0.63
2:F:19:DC:C5'	3:B:531:LYS:HZ1	2.07	0.63
2:D:19:DC:C2'	3:A:531:LYS:NZ	2.60	0.62
3:A:535:LEU:O	3:A:539:PHE:CD1	2.53	0.62
2:D:19:DC:OP2	2:D:19:DC:H6	1.82	0.62
3:B:498:LEU:N	3:B:568:LEU:O	2.32	0.62
3:B:504:LEU:HD12	3:B:525:ILE:HD11	1.81	0.62
1:C:8:DT:H4'	3:A:622:LEU:HA	0.80	0.62
2:F:20:DA:H4'	3:B:606:MET:HG3	1.81	0.62
3:B:698:ARG:HG3	3:B:811:TYR:HB3	1.80	0.62
1:C:8:DT:OP1	3:A:624:THR:N	2.33	0.62
1:C:15:DG:N1	1:C:16:DG:C6	2.67	0.62
1:C:24:DT:C3'	1:C:25:DT:P	2.86	0.62
2:D:11:DG:C2	2:D:12:DC:C2	2.87	0.62
3:B:701:PRO:HG3	3:B:811:TYR:CB	2.29	0.62
1:C:9:DG:C6	1:C:10:DG:C6	2.88	0.62
3:A:310:LEU:HD22	3:A:400:PRO:HA	1.82	0.62
3:A:458:ARG:CZ	3:A:764:LEU:CD1	2.77	0.62
3:A:662:GLY:HA3	3:A:680:ARG:HG3	1.82	0.62
3:B:696:LEU:HG	3:B:742:VAL:HG13	1.81	0.62
3:B:1039:LEU:HB3	3:B:1040:PRO:HD2	1.82	0.62
3:B:665:LYS:HB2	3:B:832:LYS:HZ1	1.64	0.62
3:A:504:LEU:HD12	3:A:525:ILE:HD11	1.81	0.62
2:D:19:DC:H5''	3:A:531:LYS:HZ3	1.63	0.61
1:E:10:DG:C4'	3:B:576:ALA:HB2	2.28	0.61
2:F:14:DA:OP2	2:F:14:DA:H8	1.83	0.61
3:A:701:PRO:HD3	3:A:811:TYR:CB	2.28	0.61
3:A:1013:HIS:CE1	3:A:1073:GLU:CA	2.83	0.61
3:B:458:ARG:CD	3:B:764:LEU:HD21	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:666:GLY:HA3	3:B:843:LEU:CD1	2.30	0.61
1:E:16:DG:H1'	1:E:17:DC:H5'	1.82	0.61
3:A:458:ARG:NH1	3:A:764:LEU:HD21	1.90	0.61
3:A:775:GLU:CD	3:B:781:ARG:NE	2.45	0.61
3:B:832:LYS:N	3:B:839:PHE:CZ	2.68	0.61
3:A:1013:HIS:HE1	3:A:1073:GLU:CA	2.13	0.61
3:A:1013:HIS:O	3:A:1016:LEU:N	2.29	0.61
3:B:996:ILE:CD1	3:B:1017:ARG:CG	2.76	0.61
1:C:14:DT:C2	2:D:14:DA:N1	2.67	0.61
1:E:22:DG:H2''	1:E:23:DT:OP2	1.99	0.61
3:A:695:SER:OG	3:A:743:TYR:HE2	1.82	0.61
3:B:492:ILE:HG13	3:B:580:VAL:HG23	1.68	0.61
3:B:535:LEU:O	3:B:539:PHE:CD1	2.53	0.61
3:A:696:LEU:HD23	3:A:742:VAL:HG13	1.82	0.61
3:A:776:GLU:HB2	3:B:775:GLU:HG3	1.81	0.61
3:A:1034:GLU:OE1	3:A:1170:GLY:HA2	2.00	0.61
3:B:458:ARG:NH2	3:B:764:LEU:CD1	2.60	0.61
3:B:662:GLY:HA3	3:B:680:ARG:HG3	1.81	0.61
3:A:999:LEU:CB	3:A:1014:PRO:HG3	2.31	0.61
1:C:8:DT:H4'	3:A:622:LEU:HD23	1.82	0.61
3:A:696:LEU:CD2	3:A:742:VAL:CG2	2.58	0.61
3:B:455:ASN:CG	3:B:760:GLY:HA3	2.26	0.61
3:B:458:ARG:NH1	3:B:764:LEU:HD21	2.14	0.61
3:B:745:GLU:OE1	3:B:814:ASN:HA	2.00	0.61
1:C:12:DA:H1'	1:C:13:DC:H5'	1.81	0.61
3:A:840:MET:HE2	3:A:843:LEU:HD12	1.83	0.61
3:A:1039:LEU:HB3	3:A:1040:PRO:HD2	1.82	0.61
1:C:12:DA:H1'	1:C:13:DC:C5'	2.31	0.60
3:A:742:VAL:H	3:A:746:GLN:NE2	1.99	0.60
3:B:496:GLY:O	3:B:569:ASN:OD1	2.18	0.60
3:A:424:ARG:NH1	5:A:1222:DTP:O4'	2.34	0.60
3:A:574:VAL:CG2	3:A:601:VAL:HG23	2.18	0.60
3:B:252:LYS:HD2	3:B:257:MET:HE3	1.84	0.60
3:B:840:MET:HE2	3:B:843:LEU:HD12	1.83	0.60
2:D:20:DA:H4'	3:A:606:MET:HG3	1.82	0.60
3:A:777:MET:HA	3:A:777:MET:HE2	1.82	0.60
3:B:777:MET:HE2	3:B:777:MET:HA	1.82	0.60
3:B:812:GLY:C	3:B:813:PHE:CB	2.74	0.60
1:C:8:DT:H5''	3:A:622:LEU:HD22	1.66	0.60
3:A:1024:VAL:CG2	3:A:1200:PRO:CG	2.79	0.60
3:B:492:ILE:HG13	3:B:580:VAL:HG21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:425:GLY:HA2	5:A:1222:DTP:O1B	2.00	0.60
3:A:698:ARG:O	3:A:701:PRO:CG	2.50	0.60
3:B:448:LEU:HD22	3:B:816:SER:CA	2.32	0.60
3:B:667:VAL:HA	3:B:828:THR:CG2	2.31	0.60
3:A:170:LEU:HD21	3:A:205:LEU:HD21	1.84	0.60
3:A:493:GLY:N	3:A:602:THR:HB	2.16	0.60
3:A:667:VAL:HA	3:A:828:THR:CG2	2.31	0.60
3:B:1035:PHE:CA	3:B:1170:GLY:HA3	2.21	0.60
1:E:14:DT:N3	2:F:15:DG:N1	2.50	0.60
3:A:575:HIS:CG	3:A:578:GLY:CA	2.83	0.60
3:B:51:PHE:HD2	3:B:603:GLN:HB3	1.66	0.60
3:B:665:LYS:HG2	3:B:860:ASP:OD1	1.96	0.60
3:B:828:THR:O	3:B:839:PHE:CE1	2.54	0.60
3:B:1035:PHE:HD1	3:B:1170:GLY:C	2.09	0.60
3:A:252:LYS:HD2	3:A:257:MET:HE3	1.83	0.60
3:A:697:TYR:CZ	3:A:702:MET:SD	2.92	0.60
3:A:994:ASP:CB	3:A:1017:ARG:HH22	2.13	0.60
3:B:743:TYR:HB2	3:B:746:GLN:HG3	1.83	0.60
3:A:701:PRO:CD	3:A:811:TYR:HB3	2.28	0.60
3:A:1013:HIS:O	3:A:1014:PRO:C	2.45	0.60
3:B:495:PHE:HZ	3:B:603:GLN:O	1.85	0.60
1:C:16:DG:O6	2:D:13:DC:O2	2.19	0.60
2:F:8:DA:H2"	2:F:9:DC:OP2	2.02	0.60
3:A:696:LEU:HD11	3:A:742:VAL:CG2	2.31	0.60
3:B:313:LEU:HB3	3:B:436:VAL:HG13	1.84	0.60
2:F:12:DC:C2	2:F:13:DC:C4	2.90	0.59
3:B:402:TYR:HE1	3:B:615:LEU:HD11	1.65	0.59
3:B:742:VAL:H	3:B:746:GLN:NE2	1.99	0.59
2:D:4:DA:H2"	2:D:5:DA:OP2	2.02	0.59
3:A:402:TYR:HE1	3:A:615:LEU:HD11	1.65	0.59
3:B:458:ARG:HH11	3:B:764:LEU:CD2	2.12	0.59
3:A:743:TYR:HB3	3:A:813:PHE:O	2.02	0.59
3:A:1026:SER:O	3:A:1027:CYS:HB2	2.02	0.59
3:A:1121:LEU:O	3:A:1124:VAL:N	2.35	0.59
3:B:1125:LEU:O	3:B:1126:GLU:HG2	2.01	0.59
3:B:170:LEU:HD21	3:B:205:LEU:HD21	1.83	0.59
1:C:9:DG:H21	3:A:576:ALA:HB3	1.66	0.59
1:C:10:DG:C5	1:C:11:DC:N4	2.70	0.59
3:A:495:PHE:CE1	3:A:605:ASP:HB3	2.38	0.59
3:B:471:ARG:HH12	3:B:630:GLU:CD	2.10	0.59
3:B:546:ARG:NE	3:B:547:ALA:CB	2.59	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:627:PHE:HB2	3:B:846:VAL:HG21	1.80	0.59
2:F:19:DC:OP1	3:B:531:LYS:HE2	2.02	0.59
3:A:186:LEU:HD21	3:A:245:PRO:HB2	1.84	0.59
3:A:538:ALA:C	3:A:539:PHE:HD1	2.10	0.59
3:A:845:SER:CA	3:A:879:ASP:CG	2.73	0.59
3:A:148:ALA:O	3:A:152:GLN:HB2	2.03	0.59
3:A:1034:GLU:HG2	3:A:1170:GLY:CA	2.31	0.59
3:A:745:GLU:OE2	3:A:815:LYS:N	2.36	0.59
3:A:1024:VAL:HG21	3:A:1200:PRO:CG	2.32	0.59
3:B:743:TYR:CA	3:B:813:PHE:O	2.51	0.59
3:B:743:TYR:HB3	3:B:813:PHE:O	2.03	0.59
3:B:845:SER:HA	3:B:879:ASP:OD1	2.03	0.59
3:A:575:HIS:CG	3:A:578:GLY:HA3	2.36	0.58
1:E:9:DG:C1'	1:E:10:DG:H5'	2.32	0.58
3:A:523:LYS:HZ3	3:A:1054:VAL:HG13	1.68	0.58
3:A:743:TYR:HB2	3:A:746:GLN:HG3	1.83	0.58
3:B:491:GLN:CB	3:B:574:VAL:HG13	1.90	0.58
1:E:9:DG:C6	1:E:10:DG:C6	2.91	0.58
3:A:855:ALA:N	3:A:1008:ILE:HG21	2.12	0.58
3:A:858:ILE:CD1	3:A:1008:ILE:CD1	2.81	0.58
3:B:999:LEU:CD2	3:B:1012:GLY:C	2.77	0.58
1:C:8:DT:C1'	1:C:9:DG:O5'	2.43	0.58
1:C:14:DT:C3'	3:A:509:ARG:HH12	2.17	0.58
3:B:148:ALA:O	3:B:152:GLN:HB2	2.03	0.58
2:D:19:DC:OP2	3:A:531:LYS:NZ	2.35	0.58
3:B:470:ASP:OD2	3:B:623:ARG:HA	2.03	0.58
3:B:538:ALA:C	3:B:539:PHE:HD1	2.10	0.58
3:B:666:GLY:HA2	3:B:857:TYR:HE2	1.69	0.58
3:A:701:PRO:HD3	3:A:811:TYR:CD2	2.38	0.58
3:A:832:LYS:CA	3:A:839:PHE:CE2	2.86	0.58
2:F:15:DG:H1'	2:F:16:DT:H5'	1.85	0.58
3:A:699:PRO:O	3:A:701:PRO:HD2	2.03	0.58
3:A:848:ARG:HD3	3:A:892:SER:OG	2.03	0.58
1:C:10:DG:H5''	3:A:473:ARG:NH2	2.19	0.57
2:F:19:DC:OP1	3:B:531:LYS:CE	2.51	0.57
3:A:774:VAL:HG21	3:B:781:ARG:HB2	1.85	0.57
1:C:16:DG:O6	2:D:13:DC:C2	2.57	0.57
2:F:6:DC:H2''	2:F:7:DG:OP2	2.04	0.57
3:A:238:ASP:HB3	3:A:239:PRO:C	2.29	0.57
3:A:567:GLY:C	3:A:568:LEU:CA	2.76	0.57
2:F:13:DC:H1'	2:F:14:DA:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:448:LEU:HD13	3:B:816:SER:CA	2.34	0.57
3:B:591:PRO:HG2	3:B:603:GLN:HB2	1.86	0.57
1:E:14:DT:OP2	3:B:233:LYS:HE2	2.05	0.57
3:A:521:LEU:HD21	3:A:548:GLU:CG	2.33	0.57
3:A:523:LYS:CD	3:A:1054:VAL:CG1	2.76	0.57
3:A:547:ALA:O	3:A:548:GLU:C	2.47	0.57
3:A:591:PRO:HG2	3:A:603:GLN:HB2	1.87	0.57
3:B:51:PHE:HD2	3:B:603:GLN:CB	2.17	0.57
1:C:6:DT:H2''	1:C:7:DG:OP2	2.05	0.57
2:D:18:DC:H2''	3:A:531:LYS:HE2	1.86	0.57
3:A:448:LEU:HD22	3:A:816:SER:CA	2.35	0.57
3:A:692:ALA:HA	3:A:743:TYR:OH	2.04	0.57
1:E:13:DC:C1'	1:E:14:DT:H5''	2.33	0.57
3:A:492:ILE:CD1	3:A:616:LYS:HB2	2.31	0.57
3:A:858:ILE:CD1	3:A:1008:ILE:HD11	2.34	0.57
3:B:51:PHE:HA	3:B:603:GLN:HB3	1.87	0.57
3:B:186:LEU:HD21	3:B:245:PRO:HB2	1.85	0.57
3:B:999:LEU:CD2	3:B:1012:GLY:O	2.52	0.57
2:F:19:DC:H2'	3:B:531:LYS:HZ1	1.69	0.57
3:A:457:GLU:CD	3:A:758:SER:OG	2.47	0.57
3:A:575:HIS:CB	3:A:578:GLY:CA	2.76	0.57
3:B:54:VAL:HG23	3:B:604:TYR:OH	1.97	0.57
3:B:238:ASP:HB3	3:B:239:PRO:C	2.29	0.57
3:B:471:ARG:HH12	3:B:630:GLU:CG	2.18	0.57
3:B:539:PHE:CZ	3:B:559:ILE:HG23	2.29	0.57
3:B:699:PRO:C	3:B:811:TYR:CE1	2.61	0.57
1:E:9:DG:O5'	1:E:9:DG:H2'	2.04	0.57
3:A:851:SER:HB3	3:A:1007:GLY:HA3	1.87	0.57
3:A:1118:VAL:O	3:A:1119:TRP:CG	2.58	0.57
1:C:8:DT:H2''	1:C:9:DG:OP2	2.05	0.56
1:E:18:DC:OP1	3:B:933:ARG:CD	2.53	0.56
1:E:19:DG:H2''	1:E:20:DT:H71	1.87	0.56
3:A:539:PHE:CZ	3:A:559:ILE:HG23	2.29	0.56
3:A:695:SER:CB	3:A:743:TYR:HE2	2.17	0.56
3:B:627:PHE:CD1	3:B:846:VAL:HG21	2.40	0.56
3:A:996:ILE:CD1	3:A:1018:TYR:OH	2.53	0.56
3:B:491:GLN:CA	3:B:492:ILE:N	2.66	0.56
3:B:742:VAL:O	3:B:813:PHE:HB2	2.05	0.56
2:D:21:DOC:H5'	2:D:21:DOC:H6	1.83	0.56
3:A:455:ASN:OD1	3:A:760:GLY:CA	2.39	0.56
3:A:496:GLY:O	3:A:569:ASN:CG	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:844:LEU:CG	3:A:880:PHE:CZ	2.88	0.56
3:A:845:SER:CB	3:A:879:ASP:OD2	2.51	0.56
3:A:996:ILE:CD1	3:A:1018:TYR:CE2	2.55	0.56
3:B:406:VAL:HA	3:B:409:TYR:CE2	2.40	0.56
3:B:627:PHE:HD1	3:B:846:VAL:CG2	2.18	0.56
2:D:20:DA:H2''	2:D:21:DOC:C5'	2.18	0.56
2:F:20:DA:C2	2:F:21:DOC:C2	2.88	0.56
1:E:20:DT:H1'	1:E:21:DC:O5'	2.05	0.56
2:F:19:DC:OP2	3:B:531:LYS:HE2	2.04	0.56
3:A:1143:LYS:HG2	3:A:1147:ARG:HD2	1.88	0.56
3:B:1125:LEU:O	3:B:1126:GLU:CD	2.48	0.56
1:C:9:DG:C2	3:A:576:ALA:HB3	2.40	0.56
3:A:627:PHE:HB2	3:A:846:VAL:HG11	1.87	0.56
3:A:665:LYS:NZ	3:A:864:LEU:HD13	2.20	0.56
1:C:21:DC:H1'	1:C:22:DG:H5'	1.88	0.56
2:F:14:DA:C1'	2:F:15:DG:C8	2.86	0.56
3:B:402:TYR:HE1	3:B:615:LEU:CD1	2.19	0.56
3:B:703:GLU:O	3:B:706:PRO:HD2	2.06	0.56
1:E:15:DG:C1'	1:E:16:DG:H5'	2.36	0.56
3:A:492:ILE:HD11	3:A:616:LYS:CB	2.30	0.56
3:A:498:LEU:HB2	3:A:568:LEU:C	2.30	0.56
3:B:54:VAL:HG21	3:B:612:LEU:HD11	1.87	0.56
3:B:711:ARG:O	3:B:714:GLY:N	2.39	0.56
3:A:1028:THR:HG22	3:A:1031:GLU:H	1.71	0.56
3:B:51:PHE:CD2	3:B:603:GLN:HG2	2.40	0.56
3:B:469:SER:HA	3:B:625:LEU:HB3	1.88	0.56
1:C:14:DT:O2	2:D:15:DG:N2	2.39	0.55
3:A:406:VAL:HA	3:A:409:TYR:CE2	2.40	0.55
3:A:407:GLN:HG3	3:A:436:VAL:CG1	2.36	0.55
3:A:565:LEU:O	3:A:568:LEU:HG	2.04	0.55
3:B:458:ARG:CZ	3:B:764:LEU:HD22	2.31	0.55
3:B:897:VAL:HG21	3:B:938:LEU:HD13	1.88	0.55
2:D:5:DA:C2'	2:D:6:DC:OP2	2.48	0.55
3:A:402:TYR:HE1	3:A:615:LEU:CD1	2.19	0.55
3:A:703:GLU:O	3:A:706:PRO:HD2	2.06	0.55
3:A:547:ALA:C	3:A:549:MET:H	2.13	0.55
3:B:424:ARG:HD3	5:B:1222:DTP:H4'	1.85	0.55
1:C:21:DC:H2''	1:C:22:DG:OP2	2.05	0.55
2:D:12:DC:C2	2:D:13:DC:C2	2.94	0.55
2:F:9:DC:C2	2:F:10:DG:C8	2.94	0.55
3:A:495:PHE:CD1	3:A:605:ASP:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:638:SER:CB	3:A:838:GLU:OE1	2.54	0.55
3:B:1035:PHE:HE1	3:B:1172:ALA:N	2.03	0.55
1:C:8:DT:C4	1:C:9:DG:C6	2.94	0.55
1:C:9:DG:H2''	1:C:10:DG:OP2	2.04	0.55
1:E:24:DT:H2''	1:E:25:DT:OP2	2.07	0.55
3:A:492:ILE:HG12	3:A:609:VAL:HG11	1.88	0.55
3:A:549:MET:HG2	3:A:559:ILE:HD12	1.89	0.55
3:A:574:VAL:HG21	3:A:601:VAL:CG2	2.20	0.55
1:C:9:DG:C2	3:A:576:ALA:HB2	2.42	0.55
2:D:12:DC:C5	2:D:13:DC:N4	2.73	0.55
2:D:12:DC:C6	2:D:13:DC:C4	2.95	0.55
2:F:14:DA:C4	2:F:15:DG:N7	2.75	0.55
3:A:897:VAL:HG21	3:A:938:LEU:HD13	1.88	0.55
3:B:238:ASP:HB3	3:B:239:PRO:CA	2.36	0.55
3:B:1035:PHE:CA	3:B:1170:GLY:CA	2.83	0.55
2:D:11:DG:H2''	2:D:12:DC:C6	2.42	0.55
3:A:665:LYS:HD3	3:A:860:ASP:HB3	1.89	0.55
3:B:711:ARG:HE	3:B:716:GLU:HG2	1.71	0.55
3:A:523:LYS:HZ3	3:A:1054:VAL:HG22	1.71	0.55
3:A:828:THR:O	3:A:839:PHE:CZ	2.60	0.55
3:B:495:PHE:CZ	3:B:603:GLN:O	2.60	0.55
3:B:549:MET:HG2	3:B:559:ILE:HD12	1.89	0.55
3:B:835:TYR:O	3:B:839:PHE:CB	2.55	0.55
3:A:458:ARG:NE	3:A:764:LEU:HD11	2.22	0.55
3:B:1126:GLU:CG	3:B:1205:PHE:HE2	2.20	0.55
1:E:8:DT:O3'	3:B:622:LEU:HA	2.06	0.54
3:A:238:ASP:HB3	3:A:239:PRO:CA	2.36	0.54
1:C:14:DT:O2	2:D:14:DA:C2	2.60	0.54
3:B:407:GLN:HG3	3:B:436:VAL:CG1	2.36	0.54
3:B:455:ASN:ND2	3:B:760:GLY:HA3	2.20	0.54
3:B:812:GLY:C	3:B:813:PHE:HD1	2.15	0.54
3:B:1143:LYS:HG2	3:B:1147:ARG:HD2	1.88	0.54
2:D:19:DC:C5'	3:A:531:LYS:NZ	2.71	0.54
3:A:458:ARG:HH21	3:A:764:LEU:HD13	1.65	0.54
3:B:665:LYS:NZ	3:B:864:LEU:CD1	2.67	0.54
3:B:831:VAL:HG11	3:B:839:PHE:CD1	2.19	0.54
1:C:9:DG:N2	3:A:576:ALA:HB3	2.22	0.54
3:B:547:ALA:O	3:B:548:GLU:C	2.49	0.54
3:B:699:PRO:HG2	3:B:811:TYR:HE2	1.73	0.54
1:C:8:DT:OP2	3:A:623:ARG:CG	2.55	0.54
1:C:16:DG:N2	2:D:14:DA:H5'	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:DG:H2''	1:E:11:DC:C6	2.42	0.54
3:B:51:PHE:CD2	3:B:603:GLN:CG	2.90	0.54
3:B:492:ILE:HG12	3:B:609:VAL:HG11	1.89	0.54
3:B:699:PRO:HB2	3:B:811:TYR:CZ	2.42	0.54
3:B:866:ILE:CG2	3:B:867:PRO:O	2.52	0.54
1:C:9:DG:P	3:A:621:GLY:C	2.87	0.54
3:A:1028:THR:HG22	3:A:1031:GLU:CG	2.36	0.54
3:B:424:ARG:NH2	5:B:1222:DTP:O4'	2.41	0.54
2:F:14:DA:P	2:F:14:DA:H2'	2.48	0.54
3:A:590:VAL:CG1	3:A:602:THR:HG23	2.38	0.54
3:A:743:TYR:HD2	3:A:813:PHE:HB3	1.73	0.54
1:E:15:DG:N1	2:F:14:DA:C2	2.76	0.54
3:A:547:ALA:HA	3:A:550:GLU:OE1	2.08	0.54
1:C:8:DT:O3'	3:A:622:LEU:C	2.50	0.54
1:C:11:DC:H2''	1:C:12:DA:OP2	2.07	0.54
1:E:23:DT:H1'	1:E:24:DT:O5'	2.08	0.54
2:F:21:DOC:OP1	3:B:616:LYS:NZ	2.33	0.54
3:A:321:ARG:NH2	3:A:440:ASN:HD21	1.99	0.54
3:A:788:ALA:HB1	3:A:793:VAL:HG23	1.90	0.54
3:B:471:ARG:HH12	3:B:630:GLU:HG2	1.71	0.54
3:B:666:GLY:CA	3:B:857:TYR:HE2	2.21	0.54
3:B:788:ALA:HB1	3:B:793:VAL:HG23	1.90	0.54
1:E:8:DT:C5'	3:B:622:LEU:HD21	2.25	0.53
1:C:14:DT:C2	2:D:15:DG:C2	2.96	0.53
3:A:441:ILE:HD12	3:A:823:LEU:HD12	1.91	0.53
3:B:310:LEU:HD22	3:B:400:PRO:HA	1.89	0.53
3:A:497:SER:HA	3:A:569:ASN:OD1	2.09	0.53
3:A:848:ARG:HE	3:A:879:ASP:CG	2.16	0.53
3:B:535:LEU:HB2	3:B:563:MET:HB3	1.90	0.53
1:C:13:DC:H2''	1:C:14:DT:C5'	2.38	0.53
1:E:15:DG:C2	1:E:16:DG:C4	2.96	0.53
3:B:840:MET:HG2	3:B:861:ALA:HB2	1.91	0.53
1:C:9:DG:O5'	1:C:9:DG:H2'	2.08	0.53
1:E:12:DA:H2''	1:E:13:DC:OP2	2.06	0.53
3:A:535:LEU:HB2	3:A:563:MET:HB3	1.90	0.53
3:A:575:HIS:CB	3:A:578:GLY:N	2.70	0.53
3:A:1034:GLU:CD	3:A:1170:GLY:CA	2.80	0.53
2:D:6:DC:C2'	2:D:7:DG:OP2	2.41	0.53
3:B:15:GLN:HE21	3:B:25:LEU:HB2	1.74	0.53
3:B:812:GLY:C	3:B:813:PHE:CD1	2.87	0.53
1:C:9:DG:H21	3:A:576:ALA:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:DG:N3	2:D:7:DG:N2	2.57	0.53
1:E:9:DG:O5'	1:E:9:DG:C2'	2.57	0.53
3:B:1034:GLU:O	3:B:1169:PHE:O	2.25	0.53
2:D:19:DC:P	3:A:531:LYS:CE	2.96	0.53
3:A:840:MET:HG2	3:A:861:ALA:HB2	1.91	0.53
3:A:1013:HIS:HE1	3:A:1073:GLU:CB	2.01	0.53
3:B:590:VAL:CG1	3:B:602:THR:HG23	2.38	0.53
2:D:19:DC:P	3:A:531:LYS:HZ1	2.29	0.53
1:E:12:DA:H1'	1:E:13:DC:H5'	1.90	0.53
2:D:18:DC:H3'	3:A:499:ALA:HB2	1.89	0.53
3:A:996:ILE:HD11	3:A:1018:TYR:OH	2.08	0.53
3:A:982:VAL:HG13	3:A:982:VAL:O	2.09	0.52
3:A:1028:THR:O	3:A:1028:THR:HG23	2.09	0.52
2:D:12:DC:C6	2:D:12:DC:O5'	2.62	0.52
2:D:14:DA:H1'	2:D:15:DG:O5'	2.10	0.52
3:A:321:ARG:NH1	3:A:434:TYR:O	2.41	0.52
3:A:574:VAL:HG22	3:A:601:VAL:HG22	0.53	0.52
3:A:1024:VAL:HG22	3:A:1200:PRO:CD	2.30	0.52
3:B:399:PHE:N	3:B:400:PRO:CD	2.72	0.52
3:B:1029:ILE:HG12	3:B:1072:ASP:CG	2.33	0.52
1:C:9:DG:OP1	3:A:621:GLY:C	2.52	0.52
3:A:399:PHE:N	3:A:400:PRO:CD	2.72	0.52
3:A:1039:LEU:HB3	3:A:1040:PRO:CD	2.39	0.52
3:B:535:LEU:HD22	3:B:559:ILE:HG23	1.92	0.52
3:B:840:MET:HE2	3:B:840:MET:HA	1.92	0.52
3:B:1140:LEU:CB	3:B:1143:LYS:HD2	2.38	0.52
3:A:535:LEU:HD22	3:A:559:ILE:HG23	1.92	0.52
3:A:773:ARG:NH1	3:B:774:VAL:HG12	2.25	0.52
3:B:742:VAL:O	3:B:813:PHE:N	2.41	0.52
3:B:788:ALA:HB1	3:B:793:VAL:CG2	2.40	0.52
2:D:11:DG:H1'	2:D:12:DC:O5'	2.10	0.52
1:E:8:DT:H4'	3:B:622:LEU:CG	2.39	0.52
1:E:13:DC:C4	1:E:14:DT:C4	2.97	0.52
3:A:296:PRO:HD2	3:A:615:LEU:HD23	1.92	0.52
3:A:313:LEU:HB3	3:A:436:VAL:HG13	1.90	0.52
3:A:461:MET:HE1	3:A:615:LEU:HA	1.91	0.52
3:A:627:PHE:CE1	3:A:843:LEU:HG	2.45	0.52
3:A:840:MET:HE2	3:A:840:MET:HA	1.91	0.52
3:B:51:PHE:CE2	3:B:593:MET:SD	3.03	0.52
1:C:23:DT:H1'	1:C:24:DT:C5'	2.40	0.52
2:D:13:DC:C4	2:D:14:DA:N6	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:239:PRO:O	3:A:240:GLU:CB	2.58	0.52
3:A:920:ASP:HA	3:A:923:LYS:HE2	1.90	0.52
3:A:994:ASP:CB	3:A:1017:ARG:CZ	2.72	0.52
2:D:6:DC:H1'	2:D:7:DG:O5'	2.09	0.52
3:B:698:ARG:O	3:B:701:PRO:CG	2.57	0.52
1:C:10:DG:C5'	3:A:576:ALA:HA	2.39	0.52
1:C:15:DG:C2	1:C:16:DG:C6	2.98	0.52
2:D:14:DA:P	2:D:14:DA:H2'	2.50	0.52
1:E:15:DG:C6	2:F:14:DA:N1	2.78	0.52
3:A:15:GLN:HE21	3:A:25:LEU:HB2	1.74	0.52
3:A:665:LYS:CB	3:A:860:ASP:CG	2.78	0.52
3:A:675:MET:O	3:A:679:VAL:HG23	2.10	0.52
3:A:788:ALA:HB1	3:A:793:VAL:CG2	2.40	0.52
3:A:1034:GLU:CG	3:A:1170:GLY:HA2	2.39	0.52
3:A:1128:PRO:HA	3:A:1129:LYS:HE3	1.91	0.52
3:B:461:MET:HE1	3:B:615:LEU:HA	1.91	0.52
3:B:1126:GLU:O	3:B:1128:PRO:HD3	2.10	0.52
1:C:15:DG:N1	1:C:16:DG:O6	2.43	0.51
3:A:832:LYS:N	3:A:839:PHE:CE1	2.78	0.51
3:A:1028:THR:N	3:A:1031:GLU:OE1	2.44	0.51
3:B:994:ASP:OD2	3:B:1017:ARG:NH2	2.42	0.51
3:A:665:LYS:CD	3:A:860:ASP:HB3	2.41	0.51
3:A:744:GLN:HG3	3:A:813:PHE:HA	1.91	0.51
3:A:773:ARG:HH12	3:B:774:VAL:HB	1.76	0.51
3:B:982:VAL:O	3:B:982:VAL:HG13	2.09	0.51
2:D:18:DC:H5'	3:A:499:ALA:CB	2.39	0.51
3:A:424:ARG:CZ	5:A:1222:DTP:C3'	2.88	0.51
3:B:493:GLY:HA3	3:B:602:THR:O	2.09	0.51
3:B:920:ASP:HA	3:B:923:LYS:HE2	1.90	0.51
3:A:80:ARG:N	3:A:128:ASP:OD1	2.44	0.51
3:B:294:ARG:NH1	3:B:612:LEU:O	2.40	0.51
3:B:1039:LEU:HB3	3:B:1040:PRO:CD	2.39	0.51
1:C:9:DG:O5'	1:C:9:DG:C2'	2.57	0.51
2:D:9:DC:C1'	2:D:10:DG:C5'	2.80	0.51
3:B:80:ARG:N	3:B:128:ASP:OD1	2.44	0.51
3:B:848:ARG:NE	3:B:879:ASP:CG	2.53	0.51
1:E:8:DT:H3'	1:E:8:DT:P	2.50	0.51
3:A:458:ARG:HH11	3:A:764:LEU:CD2	2.12	0.51
3:B:239:PRO:O	3:B:240:GLU:CB	2.58	0.51
3:B:447:GLY:N	3:B:815:LYS:NZ	2.40	0.51
3:B:548:GLU:C	3:B:550:GLU:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:DC:C4	2:F:13:DC:N4	2.78	0.51
3:A:727:GLU:OE2	3:A:731:ARG:NH1	2.44	0.51
3:B:495:PHE:HD1	3:B:605:ASP:HB3	1.75	0.51
3:B:727:GLU:OE2	3:B:731:ARG:NH1	2.44	0.51
1:E:8:DT:H3'	3:B:623:ARG:H	1.72	0.51
1:E:18:DC:O5'	1:E:18:DC:H6	1.94	0.51
3:A:744:GLN:H	3:A:813:PHE:C	2.19	0.51
3:A:1012:GLY:HA2	3:A:1013:HIS:HB2	1.92	0.51
3:B:1124:VAL:O	3:B:1125:LEU:C	2.54	0.51
3:A:447:GLY:H	3:A:815:LYS:NZ	2.09	0.51
2:D:21:DOC:C2'	5:A:1222:DTP:H4'	2.41	0.51
1:E:8:DT:H3'	1:E:8:DT:OP1	2.11	0.51
1:E:9:DG:H2'	1:E:9:DG:P	2.50	0.51
1:E:9:DG:H3'	3:B:621:GLY:HA3	1.92	0.51
3:B:675:MET:O	3:B:679:VAL:HG23	2.10	0.51
1:C:15:DG:H5''	3:A:509:ARG:NH2	2.26	0.50
3:A:776:GLU:HB2	3:B:775:GLU:CG	2.40	0.50
3:A:844:LEU:HD13	3:A:880:PHE:CZ	2.46	0.50
3:B:424:ARG:NH1	5:B:1222:DTP:O4'	2.44	0.50
3:B:1035:PHE:CE1	3:B:1172:ALA:HA	2.46	0.50
3:B:1035:PHE:HE1	3:B:1172:ALA:HA	1.76	0.50
1:E:8:DT:H2'	1:E:8:DT:OP2	2.11	0.50
2:F:15:DG:H2''	2:F:16:DT:O5'	2.11	0.50
3:A:698:ARG:HG3	3:A:701:PRO:HD2	1.93	0.50
1:C:16:DG:O6	2:D:13:DC:N3	2.44	0.50
2:F:14:DA:O5'	2:F:14:DA:C8	2.65	0.50
3:A:294:ARG:NH1	3:A:612:LEU:O	2.42	0.50
3:A:397:MET:HE2	3:A:399:PHE:HE1	1.75	0.50
1:E:21:DC:H2''	1:E:22:DG:OP2	2.11	0.50
3:A:424:ARG:CZ	5:A:1222:DTP:C4'	2.89	0.50
3:A:473:ARG:NH1	3:A:477:ILE:HD11	2.26	0.50
3:A:832:LYS:CA	3:A:839:PHE:CD2	2.94	0.50
3:B:58:LYS:CB	3:B:287:ILE:HD11	2.34	0.50
2:D:12:DC:O5'	2:D:12:DC:H6	1.94	0.50
3:B:51:PHE:CE2	3:B:603:GLN:CG	2.91	0.50
1:C:9:DG:N2	3:A:576:ALA:CB	2.75	0.50
3:A:745:GLU:OE2	3:A:814:ASN:CA	2.57	0.50
3:A:1013:HIS:O	3:A:1015:VAL:N	2.44	0.50
3:B:699:PRO:O	3:B:701:PRO:CD	2.59	0.50
3:B:812:GLY:CA	3:B:813:PHE:N	2.75	0.50
3:B:1181:VAL:HG11	3:B:1185:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:DG:C2	1:C:23:DT:C2	3.00	0.50
3:A:865:GLY:O	3:A:866:ILE:CD1	2.59	0.50
3:A:1026:SER:OG	3:A:1046:LEU:HG	2.12	0.50
3:B:473:ARG:NH1	3:B:477:ILE:HD11	2.26	0.50
1:C:9:DG:C2	2:D:20:DA:N1	2.80	0.50
1:C:8:DT:P	1:C:8:DT:H3'	2.52	0.50
1:C:14:DT:O2	2:D:14:DA:H2	1.94	0.50
2:D:18:DC:C2'	2:D:19:DC:OP2	2.55	0.50
1:E:15:DG:C6	1:E:16:DG:C6	3.00	0.50
2:F:19:DC:OP2	2:F:19:DC:H6	1.93	0.50
3:A:1140:LEU:H	3:A:1143:LYS:HD2	1.77	0.50
3:B:58:LYS:HZ1	3:B:608:ALA:HA	1.74	0.50
3:B:838:GLU:H	3:B:838:GLU:CD	2.20	0.50
2:D:21:DOC:H2''	5:A:1222:DTP:H4'	1.93	0.49
3:A:128:ASP:H	3:A:131:ILE:HG12	1.77	0.49
3:A:744:GLN:HG3	3:A:813:PHE:N	2.27	0.49
3:A:1181:VAL:HG11	3:A:1185:ALA:HB3	1.93	0.49
1:C:15:DG:C6	2:D:14:DA:C6	3.00	0.49
3:A:699:PRO:O	3:A:701:PRO:HD3	2.11	0.49
1:E:10:DG:H4'	3:B:576:ALA:CB	2.39	0.49
3:B:1140:LEU:HB2	3:B:1143:LYS:CD	2.40	0.49
2:D:21:DOC:H2''	5:A:1222:DTP:C4'	2.42	0.49
1:E:13:DC:H1'	1:E:14:DT:H5''	1.93	0.49
3:A:521:LEU:CD2	3:A:548:GLU:HG2	2.36	0.49
3:B:425:GLY:N	5:B:1222:DTP:H3'	2.27	0.49
3:A:286:PRO:HA	3:A:290:LYS:HG3	1.95	0.49
3:A:546:ARG:NH2	3:A:547:ALA:CB	2.68	0.49
1:C:15:DG:C5'	3:A:509:ARG:NH2	2.76	0.49
2:D:9:DC:H1'	2:D:10:DG:H5'	1.91	0.49
3:A:54:VAL:HG13	3:A:287:ILE:HD11	1.95	0.49
3:A:575:HIS:O	3:A:578:GLY:O	2.30	0.49
3:A:695:SER:CB	3:A:743:TYR:CE2	2.96	0.49
3:A:838:GLU:CD	3:A:838:GLU:H	2.21	0.49
3:A:851:SER:CB	3:A:895:LYS:HZ3	2.23	0.49
3:B:397:MET:HE3	3:B:459:VAL:HA	1.95	0.49
1:C:9:DG:C1'	3:A:576:ALA:HB1	2.42	0.49
2:D:11:DG:H1'	2:D:12:DC:C5'	2.43	0.49
3:A:492:ILE:CD1	3:A:616:LYS:CB	2.88	0.49
3:A:595:ASP:OD2	3:A:599:ARG:HD2	2.13	0.49
1:C:13:DC:H1'	1:C:14:DT:C5'	2.40	0.49
2:D:19:DC:P	3:A:531:LYS:HE2	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:LEU:HD13	3:A:347:GLU:HG3	1.95	0.49
3:A:1121:LEU:C	3:A:1123:GLU:N	2.69	0.49
3:B:319:LEU:HD13	3:B:347:GLU:HG3	1.95	0.49
3:B:468:PHE:C	3:B:625:LEU:HD23	2.37	0.49
3:B:537:GLU:O	3:B:539:PHE:HB2	2.13	0.49
3:B:701:PRO:HG3	3:B:811:TYR:HB3	1.93	0.49
3:B:1039:LEU:CB	3:B:1040:PRO:CD	2.91	0.49
1:C:11:DC:H4'	3:A:573:SER:OG	2.12	0.49
2:D:19:DC:OP1	3:A:531:LYS:NZ	2.42	0.49
3:A:701:PRO:HD3	3:A:811:TYR:CG	2.48	0.49
3:A:1039:LEU:CB	3:A:1040:PRO:CD	2.91	0.49
3:B:58:LYS:HZ3	3:B:608:ALA:HA	1.76	0.49
3:B:286:PRO:HA	3:B:290:LYS:HG3	1.95	0.49
1:C:15:DG:C6	2:D:14:DA:C2	2.99	0.49
2:D:12:DC:C5	2:D:13:DC:C4	3.01	0.49
1:E:10:DG:C5'	3:B:576:ALA:HB1	2.40	0.49
3:A:537:GLU:O	3:A:539:PHE:HB2	2.13	0.49
3:B:128:ASP:H	3:B:131:ILE:HG12	1.77	0.49
3:B:425:GLY:HA3	5:B:1222:DTP:O2B	2.13	0.49
3:B:574:VAL:HG13	3:B:601:VAL:HG22	1.95	0.49
3:B:701:PRO:HG3	3:B:811:TYR:HB2	1.93	0.49
1:E:9:DG:H3'	1:E:9:DG:OP1	2.13	0.48
1:E:17:DC:C3'	3:B:933:ARG:CZ	2.90	0.48
2:F:14:DA:H3'	2:F:14:DA:OP1	2.13	0.48
3:A:590:VAL:HG11	3:A:602:THR:HG23	1.95	0.48
3:A:698:ARG:HG2	3:A:701:PRO:CG	2.37	0.48
3:A:1039:LEU:HG	3:A:1040:PRO:HD3	1.95	0.48
3:B:367:LYS:O	3:B:368:ARG:HG2	2.13	0.48
3:B:575:HIS:CB	3:B:578:GLY:CA	2.68	0.48
3:B:1126:GLU:HG3	3:B:1205:PHE:HZ	1.70	0.48
1:C:15:DG:N2	2:D:14:DA:C4	2.81	0.48
3:B:181:ILE:HD13	3:B:266:TRP:CZ3	2.48	0.48
3:B:590:VAL:HG11	3:B:602:THR:HG23	1.96	0.48
3:B:1035:PHE:HE1	3:B:1172:ALA:CA	2.26	0.48
2:F:13:DC:C4	2:F:14:DA:N6	2.81	0.48
3:A:37:PRO:HB2	3:B:459:VAL:CG2	2.43	0.48
3:A:496:GLY:O	3:A:569:ASN:OD1	2.31	0.48
3:B:379:THR:HG23	3:B:382:ALA:H	1.79	0.48
3:B:1003:LYS:HD2	3:B:1096:ASP:OD2	2.13	0.48
3:B:1039:LEU:HG	3:B:1040:PRO:HD3	1.95	0.48
3:B:1050:MET:O	3:B:1070:LEU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1105:VAL:HG22	3:B:1113:VAL:HG22	1.96	0.48
3:B:1123:GLU:O	3:B:1126:GLU:CG	2.61	0.48
1:C:15:DG:OP1	3:A:509:ARG:CZ	2.61	0.48
3:A:181:ILE:HD13	3:A:266:TRP:CZ3	2.48	0.48
3:B:742:VAL:O	3:B:813:PHE:CB	2.62	0.48
2:D:14:DA:C2	2:D:15:DG:C5	3.01	0.48
2:F:11:DG:C2	2:F:12:DC:C2	3.02	0.48
3:B:448:LEU:HD13	3:B:816:SER:HB3	1.94	0.48
3:B:1128:PRO:HG2	3:B:1129:LYS:CE	2.22	0.48
1:C:8:DT:C3'	3:A:622:LEU:HA	2.40	0.48
2:F:13:DC:C2	2:F:14:DA:C5	3.01	0.48
2:F:19:DC:H2'	3:B:531:LYS:NZ	2.29	0.48
3:A:367:LYS:O	3:A:368:ARG:HG2	2.13	0.48
3:B:595:ASP:OD2	3:B:599:ARG:HD2	2.13	0.48
3:B:704:HIS:CE1	3:B:808:PHE:CZ	2.87	0.48
3:B:1173:LEU:HD13	3:B:1202:ARG:HH22	1.78	0.48
1:C:12:DA:C1'	1:C:13:DC:H5'	2.43	0.48
1:E:9:DG:H1'	3:B:576:ALA:HB1	1.94	0.48
3:A:1129:LYS:CA	3:A:1199:VAL:C	2.59	0.48
3:B:696:LEU:HG	3:B:742:VAL:CG1	2.43	0.48
3:A:234:THR:C	3:A:510:VAL:HG13	2.36	0.48
3:A:321:ARG:NH2	3:A:440:ASN:ND2	2.42	0.48
3:A:775:GLU:CD	3:B:781:ARG:CZ	2.86	0.48
1:C:12:DA:H1'	1:C:13:DC:O5'	2.14	0.48
1:E:8:DT:C4	1:E:9:DG:C6	3.02	0.48
2:D:19:DC:C2'	3:A:531:LYS:HZ1	2.26	0.48
1:E:18:DC:H2''	1:E:19:DG:OP2	2.13	0.47
3:A:1105:VAL:HG22	3:A:1113:VAL:HG22	1.96	0.47
3:B:364:GLU:HA	3:B:367:LYS:HE2	1.96	0.47
3:B:492:ILE:HA	3:B:602:THR:HG1	1.79	0.47
2:F:19:DC:P	3:B:531:LYS:CE	3.01	0.47
3:B:1053:GLU:CB	3:B:1068:PHE:HA	2.44	0.47
1:C:10:DG:C2'	1:C:11:DC:O5'	2.61	0.47
3:A:744:GLN:HG3	3:A:813:PHE:CA	2.44	0.47
3:A:776:GLU:CB	3:B:775:GLU:HG2	2.44	0.47
3:A:776:GLU:HG2	3:A:779:LYS:HD2	1.97	0.47
3:B:58:LYS:HD3	3:B:287:ILE:HD11	1.97	0.47
3:B:996:ILE:HD11	3:B:1018:TYR:CD2	2.48	0.47
1:C:8:DT:C6	1:C:9:DG:N7	2.82	0.47
3:A:364:GLU:HA	3:A:367:LYS:HE2	1.97	0.47
3:A:535:LEU:HD22	3:A:539:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1142:GLU:C	3:B:1143:LYS:HG3	2.40	0.47
3:A:493:GLY:H	3:A:602:THR:HB	1.79	0.47
3:A:1024:VAL:CG2	3:A:1200:PRO:HG2	2.39	0.47
3:A:1028:THR:C	3:A:1030:GLU:N	2.71	0.47
3:B:546:ARG:NH1	3:B:547:ALA:CB	2.64	0.47
3:B:776:GLU:HG2	3:B:779:LYS:HD2	1.97	0.47
1:E:9:DG:C2'	1:E:10:DG:H5''	2.44	0.47
1:E:17:DC:OP1	3:B:933:ARG:NH2	2.46	0.47
3:A:1050:MET:O	3:A:1070:LEU:HA	2.14	0.47
3:B:215:TYR:HB2	3:B:220:ASP:HB2	1.96	0.47
3:B:524:LEU:HB2	3:B:545:LEU:HD11	1.97	0.47
3:B:539:PHE:CE2	3:B:559:ILE:CG2	2.92	0.47
1:C:15:DG:N1	2:D:14:DA:C6	2.83	0.47
2:D:10:DG:H5'	2:D:10:DG:H8	1.79	0.47
2:D:15:DG:H2''	2:D:16:DT:O5'	2.13	0.47
2:D:19:DC:C2'	3:A:531:LYS:HZ2	2.18	0.47
3:A:379:THR:HG23	3:A:382:ALA:H	1.79	0.47
3:A:498:LEU:HB2	3:A:568:LEU:CA	2.44	0.47
3:A:523:LYS:HD3	3:A:1054:VAL:HG11	1.90	0.47
3:A:524:LEU:HB2	3:A:545:LEU:HD11	1.97	0.47
3:A:776:GLU:CG	3:B:774:VAL:HG12	2.39	0.47
3:B:666:GLY:HA2	3:B:857:TYR:CE2	2.47	0.47
3:B:696:LEU:HD11	3:B:742:VAL:HG21	1.95	0.47
3:B:743:TYR:HA	3:B:813:PHE:O	2.13	0.47
3:B:1125:LEU:O	3:B:1126:GLU:HB3	2.13	0.47
3:B:1140:LEU:HD12	3:B:1143:LYS:HZ2	1.73	0.47
3:A:546:ARG:NH1	3:A:547:ALA:CB	2.66	0.47
3:B:996:ILE:HD11	3:B:1018:TYR:CE2	2.49	0.47
3:A:1053:GLU:CB	3:A:1068:PHE:HA	2.44	0.47
3:A:1121:LEU:O	3:A:1123:GLU:N	2.47	0.47
3:B:528:GLN:HB3	3:B:533:LYS:HE3	1.97	0.47
2:D:21:DOC:C3'	5:A:1222:DTP:C4'	2.93	0.47
2:F:17:DG:H2''	2:F:18:DC:C6	2.50	0.47
3:A:294:ARG:HD3	3:A:614:LEU:HD21	1.96	0.47
3:A:851:SER:CB	3:A:895:LYS:NZ	2.74	0.47
3:A:1173:LEU:HD13	3:A:1202:ARG:HH22	1.78	0.47
3:B:1035:PHE:CD1	3:B:1171:GLU:C	2.89	0.47
3:B:1036:VAL:O	3:B:1037:ARG:C	2.58	0.47
1:C:15:DG:C6	1:C:16:DG:O6	2.68	0.46
1:E:14:DT:C3'	3:B:509:ARG:NH2	2.78	0.46
3:A:1140:LEU:HD12	3:A:1143:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:999:LEU:CD2	3:B:1013:HIS:N	2.78	0.46
3:B:1184:GLU:H	3:B:1184:GLU:HG3	1.52	0.46
1:C:14:DT:C2	2:D:15:DG:N1	2.84	0.46
1:C:24:DT:H1'	1:C:25:DT:H5'	1.98	0.46
2:D:10:DG:H2''	2:D:11:DG:O4'	2.15	0.46
3:B:402:TYR:CE2	3:B:462:PRO:HG2	2.50	0.46
3:B:492:ILE:HA	3:B:602:THR:CB	2.45	0.46
3:B:535:LEU:HD22	3:B:539:PHE:CZ	2.50	0.46
3:B:698:ARG:CG	3:B:811:TYR:HB3	2.45	0.46
3:B:1036:VAL:HG13	3:B:1043:PRO:HG2	1.97	0.46
3:A:54:VAL:CG1	3:A:287:ILE:HD11	2.45	0.46
3:A:1035:PHE:CE1	3:A:1171:GLU:O	2.68	0.46
3:B:696:LEU:HD11	3:B:742:VAL:CG2	2.45	0.46
3:B:1123:GLU:O	3:B:1126:GLU:HG2	2.16	0.46
3:A:539:PHE:CE2	3:A:559:ILE:CG2	2.92	0.46
3:A:627:PHE:CD1	3:A:843:LEU:HA	2.49	0.46
3:B:425:GLY:HA2	5:B:1222:DTP:O1B	2.15	0.46
3:B:627:PHE:CD1	3:B:846:VAL:CG2	2.97	0.46
3:B:744:GLN:HG3	3:B:813:PHE:C	2.41	0.46
1:E:8:DT:OP1	3:B:623:ARG:HB2	2.14	0.46
3:A:215:TYR:HB2	3:A:220:ASP:HB2	1.97	0.46
3:B:321:ARG:HG2	3:B:434:TYR:CE2	2.51	0.46
3:B:492:ILE:N	3:B:580:VAL:HG23	2.31	0.46
1:C:8:DT:C4'	3:A:623:ARG:N	2.73	0.46
3:A:844:LEU:CB	3:A:880:PHE:CG	2.85	0.46
3:A:1034:GLU:HG2	3:A:1170:GLY:HA2	1.94	0.46
3:B:139:LEU:O	3:B:176:ARG:HD2	2.16	0.46
3:B:448:LEU:HD23	3:B:815:LYS:HD3	1.98	0.46
3:B:665:LYS:HD3	3:B:860:ASP:CA	2.41	0.46
1:C:21:DC:H1'	1:C:22:DG:C5'	2.45	0.46
2:D:12:DC:H1'	2:D:13:DC:O4'	2.16	0.46
3:B:1072:ASP:C	3:B:1074:THR:H	2.23	0.46
1:C:16:DG:C5	1:C:17:DC:C4	3.04	0.46
2:D:11:DG:H2''	2:D:12:DC:OP2	2.15	0.46
2:D:21:DOC:C2'	3:A:424:ARG:HH11	2.03	0.46
3:A:236:LEU:O	3:A:241:ARG:NE	2.48	0.46
3:A:523:LYS:NZ	3:A:1054:VAL:CG2	2.76	0.46
3:A:828:THR:O	3:A:839:PHE:CE1	2.69	0.46
3:B:695:SER:HB2	3:B:742:VAL:CG1	2.46	0.46
1:E:12:DA:H1'	1:E:13:DC:C5'	2.45	0.46
2:F:18:DC:C2'	2:F:19:DC:OP2	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:236:LEU:O	3:B:241:ARG:NE	2.48	0.46
1:C:8:DT:OP2	3:A:623:ARG:HG3	2.15	0.46
2:D:14:DA:C2	2:D:15:DG:C4	3.04	0.46
1:E:14:DT:C2	2:F:15:DG:C2	3.04	0.46
1:C:10:DG:C4'	3:A:576:ALA:CA	2.69	0.45
2:F:13:DC:C1'	2:F:14:DA:O5'	2.58	0.45
3:A:402:TYR:CE2	3:A:462:PRO:HG2	2.50	0.45
3:A:458:ARG:CZ	3:A:764:LEU:CG	2.89	0.45
3:A:785:VAL:HG13	3:A:795:GLU:HB2	1.99	0.45
3:B:458:ARG:CZ	3:B:764:LEU:HD21	2.41	0.45
1:E:8:DT:C4'	3:B:622:LEU:CD2	2.61	0.45
3:A:57:TYR:O	3:A:61:THR:HB	2.17	0.45
3:A:1036:VAL:O	3:A:1037:ARG:C	2.58	0.45
3:B:45:THR:HG22	3:B:70:GLY:HA3	1.99	0.45
1:C:12:DA:H5'	3:A:573:SER:OG	2.16	0.45
2:D:18:DC:H5'	3:A:499:ALA:HB3	1.97	0.45
2:F:17:DG:H2'	2:F:18:DC:C5	2.52	0.45
2:F:19:DC:OP1	3:B:531:LYS:NZ	2.50	0.45
3:A:139:LEU:O	3:A:176:ARG:HD2	2.16	0.45
3:A:528:GLN:HB3	3:A:533:LYS:HE3	1.97	0.45
3:A:698:ARG:CG	3:A:701:PRO:HG3	2.43	0.45
1:C:6:DT:H5''	3:A:672:SER:OG	2.16	0.45
1:C:15:DG:P	3:A:509:ARG:CZ	3.05	0.45
1:E:8:DT:H1'	1:E:9:DG:C8	2.51	0.45
1:E:20:DT:H1'	1:E:21:DC:C6	2.51	0.45
3:A:546:ARG:NE	3:A:547:ALA:CB	2.64	0.45
3:A:574:VAL:HA	3:A:601:VAL:HG13	1.99	0.45
3:A:1101:VAL:HG22	3:A:1118:VAL:HG22	1.98	0.45
3:A:698:ARG:HG3	3:A:701:PRO:HG3	1.91	0.45
3:A:1036:VAL:HG13	3:A:1043:PRO:HG2	1.98	0.45
3:B:743:TYR:CB	3:B:813:PHE:O	2.64	0.45
3:A:492:ILE:N	3:A:580:VAL:HG23	2.31	0.45
3:A:862:ARG:HH21	3:A:1010:VAL:HG13	1.73	0.45
3:B:57:TYR:O	3:B:61:THR:HB	2.17	0.45
3:B:151:PRO:HB3	3:B:192:VAL:HG11	1.99	0.45
3:A:448:LEU:CD2	3:A:816:SER:HA	2.46	0.45
3:A:627:PHE:HZ	3:A:843:LEU:HG	1.71	0.45
3:A:678:THR:CG2	3:A:705:ILE:HG21	2.47	0.45
3:A:1072:ASP:C	3:A:1074:THR:H	2.23	0.45
3:B:424:ARG:HA	3:B:817:HIS:HD2	1.81	0.45
3:A:45:THR:HG22	3:A:70:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:546:ARG:NE	3:B:547:ALA:CA	2.80	0.45
1:C:20:DT:H2''	1:C:21:DC:OP2	2.17	0.45
1:C:25:DT:O2	2:D:4:DA:H2	2.00	0.45
1:E:15:DG:C2	1:E:16:DG:N3	2.84	0.45
3:A:1046:LEU:HA	3:A:1101:VAL:O	2.17	0.45
3:A:1120:THR:OG1	3:A:1121:LEU:N	2.49	0.45
1:C:7:DG:OP2	1:C:7:DG:C8	2.70	0.45
2:D:19:DC:C5'	3:A:531:LYS:HZ1	2.30	0.45
1:E:9:DG:N1	2:F:20:DA:N6	2.64	0.45
3:A:54:VAL:HG23	3:A:604:TYR:CZ	2.52	0.45
3:A:269:GLU:HB2	3:A:270:PRO:HD3	1.99	0.45
3:B:446:PHE:HB3	3:B:815:LYS:CE	2.44	0.45
2:D:12:DC:C2	2:D:13:DC:N3	2.85	0.44
2:D:19:DC:N3	2:D:20:DA:N6	2.65	0.44
2:D:21:DOC:C5'	2:D:21:DOC:C6	2.82	0.44
2:F:7:DG:H1'	2:F:8:DA:O5'	2.18	0.44
3:A:151:PRO:HB3	3:A:192:VAL:HG11	1.99	0.44
3:A:424:ARG:HB2	5:A:1222:DTP:O3'	2.17	0.44
3:A:773:ARG:HH12	3:B:774:VAL:CB	2.30	0.44
3:A:1129:LYS:N	3:A:1201:ASP:H	2.15	0.44
3:B:1035:PHE:CB	3:B:1170:GLY:HA2	2.42	0.44
3:A:835:TYR:O	3:A:839:PHE:HB2	2.16	0.44
3:B:785:VAL:HG13	3:B:795:GLU:HB2	1.98	0.44
3:B:832:LYS:CA	3:B:839:PHE:CG	2.95	0.44
3:B:1102:LEU:HD12	3:B:1119:TRP:HH2	1.83	0.44
3:B:24:LYS:HZ3	3:B:567:GLY:HA3	1.82	0.44
1:E:13:DC:N3	1:E:14:DT:C4	2.86	0.44
3:A:321:ARG:CG	3:A:434:TYR:CE2	3.00	0.44
3:A:769:MET:HE1	3:A:806:GLU:HB3	2.00	0.44
3:B:800:ARG:O	3:B:803:ASP:HB2	2.17	0.44
3:B:1046:LEU:HA	3:B:1101:VAL:O	2.17	0.44
3:B:1128:PRO:HG3	3:B:1129:LYS:HE3	0.44	0.44
1:E:18:DC:H5''	3:B:933:ARG:HB3	1.99	0.44
2:F:11:DG:H2''	2:F:12:DC:OP2	2.18	0.44
3:A:774:VAL:CA	3:B:778:GLN:CG	2.72	0.44
3:B:491:GLN:O	3:B:492:ILE:C	2.61	0.44
3:B:1126:GLU:CG	3:B:1205:PHE:CE2	2.84	0.44
3:B:1152:LEU:CB	3:B:1179:VAL:HG11	2.45	0.44
1:C:9:DG:P	1:C:9:DG:C2'	3.04	0.44
1:E:10:DG:H2''	1:E:11:DC:C5	2.53	0.44
3:B:492:ILE:CD1	3:B:616:LYS:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1034:GLU:HG2	3:B:1169:PHE:CA	2.48	0.44
3:A:367:LYS:C	3:A:368:ARG:CG	2.91	0.44
3:A:575:HIS:NE2	3:A:577:ALA:HB3	2.33	0.44
3:A:1121:LEU:O	3:A:1122:GLU:C	2.61	0.44
3:B:269:GLU:HB2	3:B:270:PRO:HD3	1.99	0.44
3:B:424:ARG:NH1	5:B:1222:DTP:C4'	2.81	0.44
2:D:19:DC:P	3:A:531:LYS:HZ3	2.31	0.44
3:A:623:ARG:HD2	3:A:846:VAL:CG1	2.48	0.44
1:C:24:DT:H2''	1:C:25:DT:O5'	2.17	0.43
3:A:1028:THR:H	3:A:1031:GLU:HB2	1.83	0.43
1:C:8:DT:H1'	1:C:9:DG:C5'	2.46	0.43
1:E:18:DC:H5''	3:B:933:ARG:CB	2.48	0.43
1:E:23:DT:C2	1:E:24:DT:C4	3.06	0.43
3:A:384:LEU:HD23	3:A:384:LEU:HA	1.91	0.43
3:A:574:VAL:CG1	3:A:601:VAL:HG22	2.47	0.43
3:A:698:ARG:O	3:A:700:GLY:C	2.60	0.43
3:A:795:GLU:HA	3:A:798:ALA:HB3	2.01	0.43
3:B:1128:PRO:HA	3:B:1200:PRO:HA	1.99	0.43
1:C:11:DC:H2''	1:C:12:DA:C8	2.52	0.43
1:E:18:DC:P	3:B:933:ARG:HB2	2.49	0.43
3:B:402:TYR:CE1	3:B:615:LEU:CD1	3.01	0.43
3:B:639:LYS:HD2	3:B:835:TYR:CD2	2.53	0.43
3:B:795:GLU:HA	3:B:798:ALA:HB3	2.00	0.43
3:B:455:ASN:CG	3:B:760:GLY:HA2	2.38	0.43
3:B:495:PHE:CD1	3:B:605:ASP:HB3	2.51	0.43
2:D:21:DOC:C3'	5:A:1222:DTP:C5'	2.87	0.43
1:E:15:DG:H2''	1:E:16:DG:OP2	2.17	0.43
3:A:425:GLY:CA	5:A:1222:DTP:O1B	2.65	0.43
3:A:696:LEU:HD21	3:A:742:VAL:CG1	2.46	0.43
1:E:10:DG:C4'	3:B:576:ALA:HB1	2.47	0.43
3:A:1035:PHE:HE1	3:A:1172:ALA:HA	1.83	0.43
3:B:467:ASP:HB3	3:B:622:LEU:HD12	1.99	0.43
3:B:840:MET:HA	3:B:840:MET:CE	2.49	0.43
1:C:14:DT:C2	2:D:15:DG:N2	2.86	0.43
2:D:19:DC:H6	3:A:531:LYS:HE2	1.82	0.43
3:A:296:PRO:HG2	3:A:581:ILE:HG22	2.01	0.43
3:A:800:ARG:O	3:A:803:ASP:HB2	2.17	0.43
3:B:458:ARG:HH12	3:B:764:LEU:HD22	1.65	0.43
3:B:492:ILE:HG12	3:B:609:VAL:HG21	2.00	0.43
3:B:999:LEU:HB2	3:B:1014:PRO:HG3	1.97	0.43
3:A:840:MET:HA	3:A:840:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:769:MET:HE1	3:B:806:GLU:HB3	2.00	0.43
1:C:9:DG:C5	1:C:10:DG:N7	2.87	0.43
1:C:15:DG:C4	1:C:16:DG:C8	3.06	0.43
2:D:14:DA:OP2	2:D:14:DA:H8	2.01	0.43
3:A:310:LEU:CD2	3:A:400:PRO:HA	2.48	0.43
3:B:441:ILE:HD13	3:B:819:ALA:C	2.44	0.43
3:B:773:ARG:O	3:B:774:VAL:C	2.62	0.43
1:E:8:DT:C1'	1:E:9:DG:C5'	2.97	0.42
2:F:5:DA:H1'	2:F:6:DC:C6	2.53	0.42
3:A:296:PRO:CG	3:A:581:ILE:HG22	2.49	0.42
3:A:428:ALA:HB3	3:A:816:SER:HB2	2.01	0.42
3:A:443:PRO:O	3:A:446:PHE:O	2.36	0.42
3:A:495:PHE:HZ	3:A:603:GLN:O	2.02	0.42
3:A:534:PRO:HA	3:A:566:GLU:OE2	2.19	0.42
3:A:627:PHE:CZ	3:A:843:LEU:CG	2.93	0.42
3:B:367:LYS:C	3:B:368:ARG:CG	2.91	0.42
3:B:443:PRO:O	3:B:446:PHE:O	2.36	0.42
3:B:1101:VAL:HG22	3:B:1118:VAL:HG22	2.00	0.42
1:E:10:DG:C2'	1:E:11:DC:C5	3.01	0.42
3:B:431:LEU:HA	3:B:443:PRO:HG3	2.01	0.42
3:B:832:LYS:CA	3:B:839:PHE:CZ	2.97	0.42
3:B:866:ILE:CG2	3:B:867:PRO:CD	2.84	0.42
1:C:14:DT:C3'	3:A:509:ARG:NH1	2.76	0.42
1:C:25:DT:O2	2:D:4:DA:C2	2.72	0.42
2:D:11:DG:H1'	2:D:12:DC:H5'	2.01	0.42
1:E:9:DG:C4'	3:B:621:GLY:N	2.81	0.42
3:A:1024:VAL:HG23	3:A:1200:PRO:CD	2.34	0.42
3:B:526:PRO:CD	3:B:538:ALA:CB	2.97	0.42
1:C:8:DT:H3'	3:A:623:ARG:CA	2.47	0.42
1:E:8:DT:C3'	1:E:8:DT:P	3.08	0.42
2:F:14:DA:C4	2:F:15:DG:C5	3.08	0.42
3:B:492:ILE:HD12	3:B:616:LYS:HG3	2.01	0.42
1:E:24:DT:C2	2:F:5:DA:H2	2.37	0.42
3:A:294:ARG:CB	3:A:614:LEU:HD23	2.46	0.42
3:B:548:GLU:O	3:B:551:LYS:N	2.45	0.42
3:B:996:ILE:HA	3:B:1014:PRO:HA	2.01	0.42
3:A:252:LYS:HB3	3:A:256:GLU:HB2	2.02	0.42
3:B:570:ARG:HA	3:B:570:ARG:HD3	1.84	0.42
3:B:999:LEU:HD21	3:B:1013:HIS:N	2.34	0.42
3:B:1192:GLU:C	3:B:1194:TYR:H	2.27	0.42
1:C:14:DT:H2''	1:C:15:DG:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:DG:H2''	2:D:12:DC:C5	2.55	0.42
2:D:19:DC:C6	3:A:531:LYS:CE	2.99	0.42
3:A:567:GLY:C	3:A:568:LEU:HA	2.45	0.42
3:A:1034:GLU:CG	3:A:1170:GLY:CA	2.96	0.42
3:B:525:ILE:HA	3:B:526:PRO:HD3	1.90	0.42
3:B:595:ASP:C	3:B:595:ASP:OD1	2.62	0.42
3:B:1035:PHE:CB	3:B:1170:GLY:CA	2.98	0.42
1:C:23:DT:H2''	1:C:24:DT:H72	2.02	0.42
1:E:6:DT:C2'	1:E:7:DG:OP2	2.58	0.42
3:A:402:TYR:CE1	3:A:615:LEU:CD1	3.01	0.42
3:A:666:GLY:HA3	3:A:843:LEU:CD1	2.50	0.42
3:A:773:ARG:O	3:A:774:VAL:C	2.62	0.42
3:B:252:LYS:HB3	3:B:256:GLU:HB2	2.01	0.42
3:B:534:PRO:HA	3:B:566:GLU:OE2	2.19	0.42
3:B:1039:LEU:HG	3:B:1040:PRO:CD	2.50	0.42
2:D:19:DC:H2''	2:D:20:DA:C8	2.55	0.42
3:A:526:PRO:CD	3:A:538:ALA:CB	2.97	0.42
3:A:594:ARG:HH11	3:A:594:ARG:HG3	1.84	0.42
3:A:752:SER:HA	3:A:757:TYR:HB2	2.02	0.42
3:A:812:GLY:C	3:A:813:PHE:N	2.78	0.42
3:A:1182:GLY:O	3:A:1183:GLU:HB2	2.20	0.42
3:B:725:HIS:HD2	3:B:797:GLU:OE2	2.03	0.42
1:C:11:DC:H6	1:C:11:DC:H2'	1.65	0.42
2:D:5:DA:H1'	2:D:6:DC:P	2.60	0.42
1:E:14:DT:O2	2:F:15:DG:C2	2.72	0.42
3:A:306:GLU:O	3:A:404:LEU:HD11	2.19	0.42
3:A:424:ARG:HB3	3:A:821:TYR:HE1	1.84	0.42
3:A:832:LYS:N	3:A:839:PHE:CZ	2.87	0.42
3:B:425:GLY:H	3:B:817:HIS:HD2	1.64	0.42
3:B:448:LEU:CD2	3:B:816:SER:HA	2.50	0.42
3:B:455:ASN:OD1	3:B:760:GLY:CA	2.61	0.42
3:B:627:PHE:CG	3:B:846:VAL:HG21	2.55	0.42
3:A:424:ARG:HD3	5:A:1222:DTP:H4'	2.01	0.41
3:A:566:GLU:C	3:A:568:LEU:N	2.77	0.41
3:A:1028:THR:CG2	3:A:1031:GLU:H	2.33	0.41
1:C:11:DC:H1'	1:C:12:DA:C8	2.55	0.41
1:E:9:DG:C5	1:E:10:DG:C5	3.08	0.41
3:A:542:GLU:HG3	3:A:545:LEU:H	1.85	0.41
3:A:1026:SER:CB	3:A:1202:ARG:NH2	2.69	0.41
3:A:1128:PRO:N	3:A:1200:PRO:HB3	2.33	0.41
3:B:666:GLY:O	3:B:843:LEU:HD21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:DC:C4'	3:A:531:LYS:HZ1	2.32	0.41
3:A:498:LEU:HD12	3:A:568:LEU:HB2	2.02	0.41
3:A:1184:GLU:H	3:A:1184:GLU:HG3	1.52	0.41
3:B:316:LEU:HD21	3:B:348:ARG:HA	2.02	0.41
3:B:457:GLU:OE2	3:B:758:SER:OG	2.36	0.41
3:B:535:LEU:CB	3:B:563:MET:HB3	2.49	0.41
3:B:594:ARG:HG3	3:B:594:ARG:HH11	1.84	0.41
3:B:708:TYR:HD1	3:B:740:ILE:HD12	1.85	0.41
3:B:994:ASP:CG	3:B:1017:ARG:NH2	2.79	0.41
3:B:1035:PHE:HB2	3:B:1170:GLY:CA	2.47	0.41
1:C:11:DC:P	1:C:11:DC:C3'	3.05	0.41
2:D:8:DA:H2''	2:D:9:DC:OP2	2.19	0.41
2:D:19:DC:H2'	3:A:531:LYS:HZ1	1.75	0.41
3:A:211:ASN:O	3:A:211:ASN:CG	2.63	0.41
3:A:725:HIS:HD2	3:A:797:GLU:OE2	2.03	0.41
3:A:858:ILE:CD1	3:A:1008:ILE:HD13	2.43	0.41
3:A:1039:LEU:HG	3:A:1040:PRO:CD	2.50	0.41
3:B:524:LEU:HD13	3:B:545:LEU:HG	2.02	0.41
3:B:699:PRO:HG2	3:B:811:TYR:CE2	2.54	0.41
3:A:316:LEU:HD21	3:A:348:ARG:HA	2.02	0.41
3:A:367:LYS:C	3:A:368:ARG:HG2	2.45	0.41
3:A:535:LEU:CB	3:A:563:MET:HB3	2.50	0.41
3:B:235:THR:HG23	3:B:510:VAL:O	2.20	0.41
3:B:252:LYS:HD2	3:B:257:MET:CE	2.50	0.41
3:B:696:LEU:CG	3:B:742:VAL:CG2	2.96	0.41
2:D:13:DC:N4	2:D:14:DA:N6	2.68	0.41
3:A:27:ASP:HA	3:A:30:LYS:HG2	2.03	0.41
3:A:1128:PRO:HB3	3:A:1129:LYS:HE3	2.03	0.41
3:B:179:ILE:HG13	3:B:200:ALA:HB2	2.03	0.41
3:B:546:ARG:NH2	3:B:547:ALA:CB	2.74	0.41
3:B:832:LYS:CB	3:B:839:PHE:HE2	2.02	0.41
1:C:8:DT:O3'	3:A:622:LEU:CA	2.69	0.41
1:C:8:DT:C4	1:C:9:DG:O6	2.74	0.41
1:C:23:DT:C1'	1:C:24:DT:O5'	2.62	0.41
3:A:431:LEU:HA	3:A:443:PRO:HG3	2.02	0.41
3:A:602:THR:HG21	3:A:609:VAL:CG2	2.51	0.41
3:B:211:ASN:O	3:B:211:ASN:CG	2.63	0.41
3:B:321:ARG:CG	3:B:434:TYR:CE2	3.03	0.41
3:B:1182:GLY:O	3:B:1183:GLU:HB2	2.21	0.41
1:C:7:DG:C1'	1:C:8:DT:O5'	2.66	0.41
2:F:17:DG:C2'	2:F:18:DC:C6	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:DA:C3'	2:F:21:DOC:H5'	2.47	0.41
3:A:390:GLU:CD	3:A:450:PHE:CD1	2.98	0.41
3:A:492:ILE:CG1	3:A:609:VAL:HG11	2.50	0.41
3:A:524:LEU:HD13	3:A:545:LEU:HG	2.03	0.41
1:C:9:DG:OP1	3:A:621:GLY:HA3	2.21	0.41
1:C:9:DG:H2'	1:C:9:DG:OP2	2.21	0.41
1:E:19:DG:C4	1:E:20:DT:C4	3.08	0.41
3:A:252:LYS:HD2	3:A:257:MET:CE	2.50	0.41
3:A:285:LEU:CB	3:A:286:PRO:CD	2.81	0.41
3:A:458:ARG:NE	3:A:764:LEU:CD1	2.84	0.41
3:A:595:ASP:OD1	3:A:595:ASP:C	2.62	0.41
3:A:858:ILE:HD13	3:A:1008:ILE:HD11	2.02	0.41
3:A:1023:GLU:HB3	3:A:1199:VAL:HG12	2.03	0.41
3:A:1192:GLU:C	3:A:1194:TYR:H	2.27	0.41
3:B:27:ASP:HA	3:B:30:LYS:HG2	2.03	0.41
3:B:367:LYS:C	3:B:368:ARG:HG2	2.45	0.41
3:B:602:THR:HG21	3:B:609:VAL:CG2	2.51	0.41
3:B:752:SER:HA	3:B:757:TYR:HB2	2.01	0.41
3:B:1034:GLU:HG2	3:B:1169:PHE:CB	2.50	0.41
3:B:1123:GLU:O	3:B:1125:LEU:O	2.39	0.41
1:C:6:DT:C5'	3:A:672:SER:OG	2.69	0.41
1:E:9:DG:H1	2:F:20:DA:N6	2.19	0.41
1:E:19:DG:C2'	1:E:20:DT:H71	2.51	0.41
3:A:285:LEU:HA	3:A:286:PRO:HD3	1.51	0.41
3:A:402:TYR:CE1	3:A:615:LEU:HD11	2.52	0.41
3:A:506:ASP:OD2	3:A:570:ARG:NH2	2.23	0.41
3:A:834:HIS:O	3:A:836:PRO:HD3	2.21	0.41
3:B:855:ALA:HA	3:B:1008:ILE:HG21	2.03	0.41
3:B:873:VAL:HG22	3:B:943:ALA:O	2.21	0.41
2:D:11:DG:H2''	2:D:12:DC:O5'	2.21	0.40
1:E:9:DG:N1	2:F:20:DA:C6	2.88	0.40
1:E:19:DG:H2''	1:E:20:DT:OP2	2.20	0.40
3:A:290:LYS:H	3:A:290:LYS:HG2	1.47	0.40
3:A:873:VAL:HG22	3:A:943:ALA:O	2.22	0.40
3:B:574:VAL:CG1	3:B:601:VAL:HG22	2.52	0.40
1:E:8:DT:P	1:E:8:DT:H2'	2.61	0.40
1:E:24:DT:H6	1:E:24:DT:H2'	1.73	0.40
3:A:546:ARG:NE	3:A:546:ARG:C	2.78	0.40
3:A:915:PHE:HA	3:A:924:ARG:HH21	1.86	0.40
3:B:271:PHE:O	3:B:274:THR:HB	2.22	0.40
3:B:602:THR:HG22	3:B:604:TYR:N	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:665:LYS:H	3:B:665:LYS:HG3	1.72	0.40
1:C:13:DC:C1'	1:C:14:DT:H5''	2.44	0.40
1:C:16:DG:O6	2:D:12:DC:O2	2.40	0.40
3:A:448:LEU:HD22	3:A:816:SER:N	2.36	0.40
3:A:776:GLU:HB3	3:B:775:GLU:HG2	2.03	0.40
3:B:526:PRO:HD3	3:B:538:ALA:CB	2.52	0.40
3:B:542:GLU:HG3	3:B:545:LEU:H	1.85	0.40
3:B:699:PRO:CB	3:B:811:TYR:CE2	3.04	0.40
1:C:22:DG:N2	1:C:23:DT:C2	2.90	0.40
3:A:492:ILE:N	3:A:580:VAL:CG2	2.84	0.40
3:B:321:ARG:HD3	3:B:434:TYR:O	2.21	0.40
3:B:698:ARG:HD2	3:B:811:TYR:HB3	2.02	0.40
3:B:763:ASP:O	3:B:767:ARG:HG2	2.22	0.40
3:B:915:PHE:HA	3:B:924:ARG:HH21	1.85	0.40
1:C:7:DG:OP2	1:C:7:DG:H8	2.05	0.40
1:C:14:DT:C4	2:D:14:DA:N6	2.79	0.40
1:C:23:DT:C2'	1:C:24:DT:H72	2.51	0.40
2:D:20:DA:H2''	2:D:21:DOC:H6	2.03	0.40
3:A:424:ARG:NH2	5:A:1222:DTP:H1'	2.37	0.40
3:A:495:PHE:HE1	3:A:605:ASP:HB3	1.85	0.40
3:A:570:ARG:HA	3:A:570:ARG:HD3	1.84	0.40
3:A:737:THR:HG21	3:A:746:GLN:HE22	1.87	0.40
3:B:492:ILE:CG1	3:B:580:VAL:HG21	2.37	0.40
3:B:666:GLY:CA	3:B:857:TYR:CE2	3.03	0.40
3:B:743:TYR:C	3:B:813:PHE:O	2.61	0.40
3:B:1042:LYS:HG2	3:B:1106:GLU:HG2	2.03	0.40

All (36) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1177:ARG:NH2	3:B:972:ARG:CA[3_655]	0.82	1.38
3:A:1154:GLU:O	3:B:157:ASP:OD2[1_655]	0.99	1.21
3:A:657:GLU:OE2	3:B:654:LYS:N[2_655]	1.00	1.20
3:A:1177:ARG:NH2	3:B:972:ARG:CB[3_655]	1.14	1.06
3:A:654:LYS:N	3:B:657:GLU:OE2[2_655]	1.22	0.98
3:A:1169:PHE:CE1	3:B:637:GLU:O[2_655]	1.36	0.84
3:A:1169:PHE:CD1	3:B:638:SER:O[2_655]	1.37	0.83
3:A:657:GLU:OE1	3:B:654:LYS:CG[2_655]	1.41	0.79
3:A:971:GLY:O	3:B:1177:ARG:NH2[3_645]	1.49	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1169:PHE:CZ	3:B:637:GLU:O[2_655]	1.57	0.63
3:A:653:PRO:C	3:B:657:GLU:OE2[2_655]	1.59	0.61
3:B:347:GLU:OE1	3:B:991:SER:OG[4_554]	1.64	0.56
3:A:1177:ARG:CZ	3:B:972:ARG:C[3_655]	1.66	0.54
3:A:657:GLU:OE2	3:B:654:LYS:CA[2_655]	1.69	0.51
3:A:1177:ARG:CZ	3:B:972:ARG:O[3_655]	1.69	0.51
3:A:1041:GLY:N	3:B:982:VAL:CG2[3_655]	1.72	0.48
3:A:1177:ARG:NE	3:B:972:ARG:C[3_655]	1.72	0.48
3:A:1177:ARG:CZ	3:B:972:ARG:CA[3_655]	1.74	0.46
3:A:1177:ARG:NH2	3:B:972:ARG:C[3_655]	1.86	0.34
3:A:653:PRO:CG	3:B:657:GLU:CG[2_655]	1.87	0.33
3:A:657:GLU:CD	3:B:654:LYS:CG[2_655]	1.88	0.32
3:A:653:PRO:CA	3:B:657:GLU:OE2[2_655]	1.94	0.26
3:A:653:PRO:CB	3:B:657:GLU:OE2[2_655]	1.95	0.25
3:A:657:GLU:OE2	3:B:653:PRO:C[2_655]	1.99	0.21
3:A:1177:ARG:NH1	3:B:972:ARG:O[3_655]	2.02	0.18
3:A:1177:ARG:CG	3:B:974:GLY:N[3_655]	2.03	0.17
3:A:1177:ARG:NE	3:B:972:ARG:O[3_655]	2.07	0.13
3:B:304:ARG:NH2	3:B:1017:ARG:CZ[4_554]	2.07	0.13
3:A:1169:PHE:CD1	3:B:638:SER:C[2_655]	2.12	0.08
3:A:971:GLY:O	3:B:1177:ARG:CZ[3_645]	2.13	0.07
3:A:654:LYS:CG	3:B:657:GLU:OE1[2_655]	2.16	0.04
3:A:654:LYS:N	3:B:657:GLU:CD[2_655]	2.17	0.03
2:D:7:DG:OP1	3:A:475:ARG:NH2[4_654]	2.18	0.02
3:A:1154:GLU:O	3:B:157:ASP:CG[1_655]	2.18	0.02
3:B:304:ARG:NH2	3:B:1017:ARG:NH2[4_554]	2.18	0.02
3:A:1154:GLU:C	3:B:157:ASP:OD2[1_655]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	1124/1220 (92%)	1006 (90%)	88 (8%)	30 (3%)	4 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	1120/1220 (92%)	1007 (90%)	82 (7%)	31 (3%)	4	24
All	All	2244/2440 (92%)	2013 (90%)	170 (8%)	61 (3%)	4	25

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	286	PRO
3	A	537	GLU
3	A	538	ALA
3	A	774	VAL
3	A	836	PRO
3	A	1013	HIS
3	A	1014	PRO
3	A	1029	ILE
3	A	1039	LEU
3	A	1127	ALA
3	A	1128	PRO
3	A	1130	ALA
3	A	1176	LEU
3	B	492	ILE
3	B	537	GLU
3	B	538	ALA
3	B	549	MET
3	B	774	VAL
3	B	866	ILE
3	B	1014	PRO
3	B	1039	LEU
3	B	1142	GLU
3	B	1176	LEU
3	A	290	LYS
3	A	291	MET
3	A	539	PHE
3	A	548	GLU
3	A	570	ARG
3	A	792	GLY
3	A	975	LEU
3	A	976	VAL
3	A	1122	GLU
3	A	1177	ARG
3	B	290	LYS
3	B	291	MET
3	B	539	PHE

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Mol	Chain	Res	Type
3	B	548	GLU
3	B	570	ARG
3	B	714	GLY
3	B	715	GLN
3	B	792	GLY
3	B	975	LEU
3	B	976	VAL
3	B	1177	ARG
3	B	836	PRO
3	B	1143	LYS
3	A	53	ALA
3	A	238	ASP
3	B	53	ALA
3	B	238	ASP
3	B	867	PRO
3	B	1193	GLY
3	A	736	GLU
3	A	977	GLY
3	A	1027	CYS
3	A	1193	GLY
3	B	736	GLU
3	B	977	GLY
3	B	1125	LEU
3	A	399	PHE
3	B	399	PHE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DOC	D	21	2,1	16,19,20	0.60	0	20,26,29	0.70	1 (5%)
2	DOC	F	21	2,1	16,19,20	0.55	0	20,26,29	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	D	21	2,1	-	2/7/18/19	0/2/2/2
2	DOC	F	21	2,1	-	2/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	21	DOC	C3'-C2'-C1'	2.24	105.45	102.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	21	DOC	C3'-C4'-C5'-O5'
2	D	21	DOC	C4'-C5'-O5'-P
2	F	21	DOC	C4'-C5'-O5'-P
2	F	21	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	21	DOC	25	0
2	F	21	DOC	16	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
5	DTP	A	1222	4	31,32,32	1.47	4 (12%)	46,50,50	1.08	3 (6%)
5	DTP	B	1222	4	31,32,32	1.46	4 (12%)	46,50,50	1.08	3 (6%)

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
5	DTP	A	1222	4	-	5/22/34/34	0/3/3/3
5	DTP	B	1222	4	-	5/22/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1222	DTP	PB-O3B	-4.70	1.54	1.59
5	B	1222	DTP	PB-O3B	-4.64	1.54	1.59
5	B	1222	DTP	O4'-C1'	-3.14	1.35	1.42
5	A	1222	DTP	O4'-C1'	-3.13	1.35	1.42
5	B	1222	DTP	PA-O2A	-2.73	1.42	1.55
5	A	1222	DTP	PA-O2A	-2.70	1.42	1.55
5	A	1222	DTP	PB-O3A	-2.52	1.56	1.59
5	B	1222	DTP	PB-O3A	-2.32	1.57	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1222	DTP	C2'-C1'-N9	-3.16	107.20	114.63
5	B	1222	DTP	C2'-C1'-N9	-3.13	107.28	114.63
5	B	1222	DTP	O3'-C3'-C4'	2.94	121.23	110.07
5	A	1222	DTP	O3'-C3'-C4'	2.93	121.17	110.07
5	A	1222	DTP	O3G-PG-O3B	-2.84	95.11	104.64
5	B	1222	DTP	O3G-PG-O3B	-2.82	95.17	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

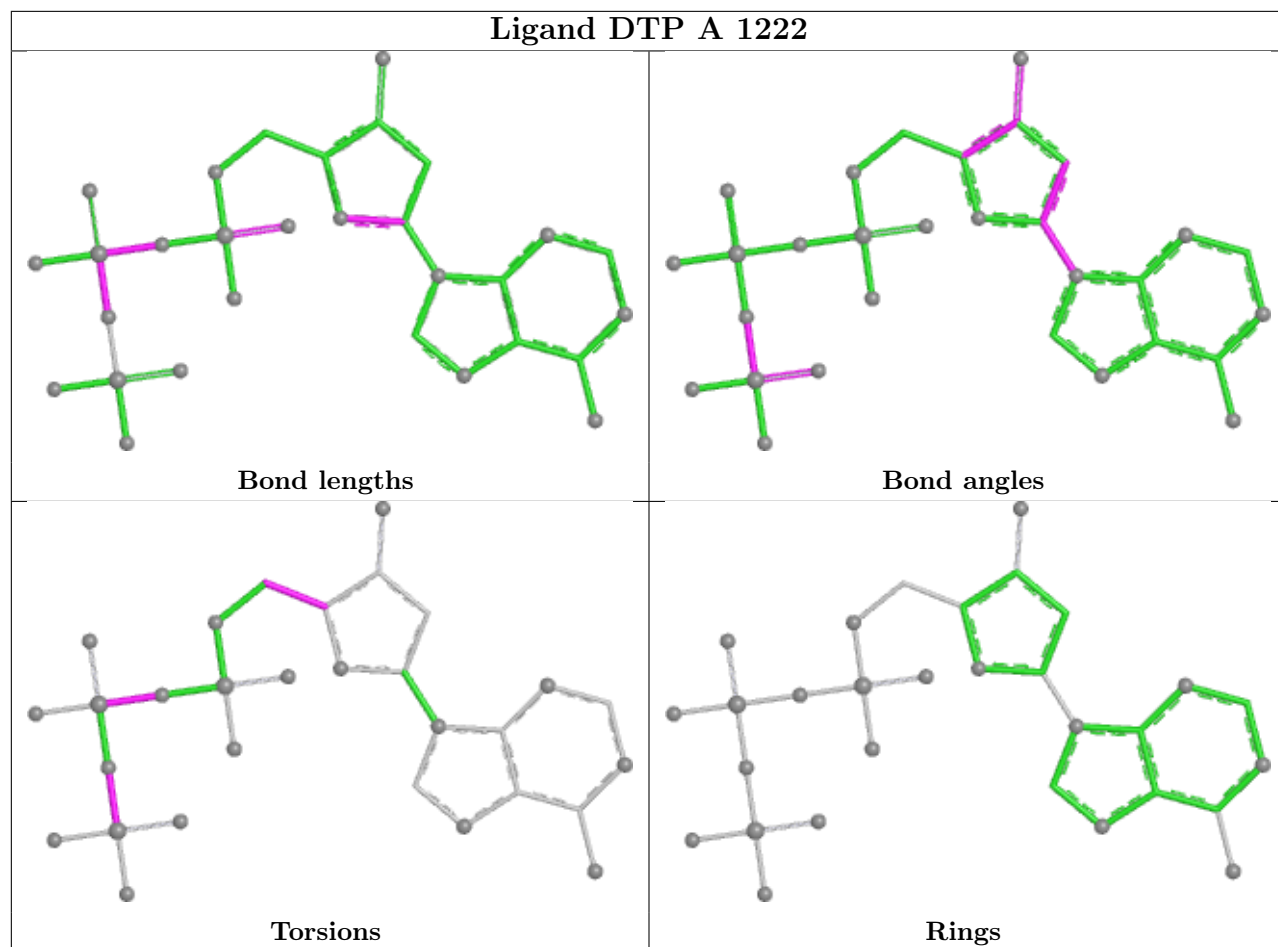
Mol	Chain	Res	Type	Atoms
5	A	1222	DTP	PB-O3B-PG-O3G
5	B	1222	DTP	PB-O3B-PG-O3G
5	A	1222	DTP	O4'-C4'-C5'-O5'
5	B	1222	DTP	O4'-C4'-C5'-O5'
5	A	1222	DTP	PA-O3A-PB-O1B
5	B	1222	DTP	PA-O3A-PB-O1B
5	B	1222	DTP	C3'-C4'-C5'-O5'
5	A	1222	DTP	C3'-C4'-C5'-O5'
5	A	1222	DTP	PA-O3A-PB-O2B
5	B	1222	DTP	PA-O3A-PB-O2B

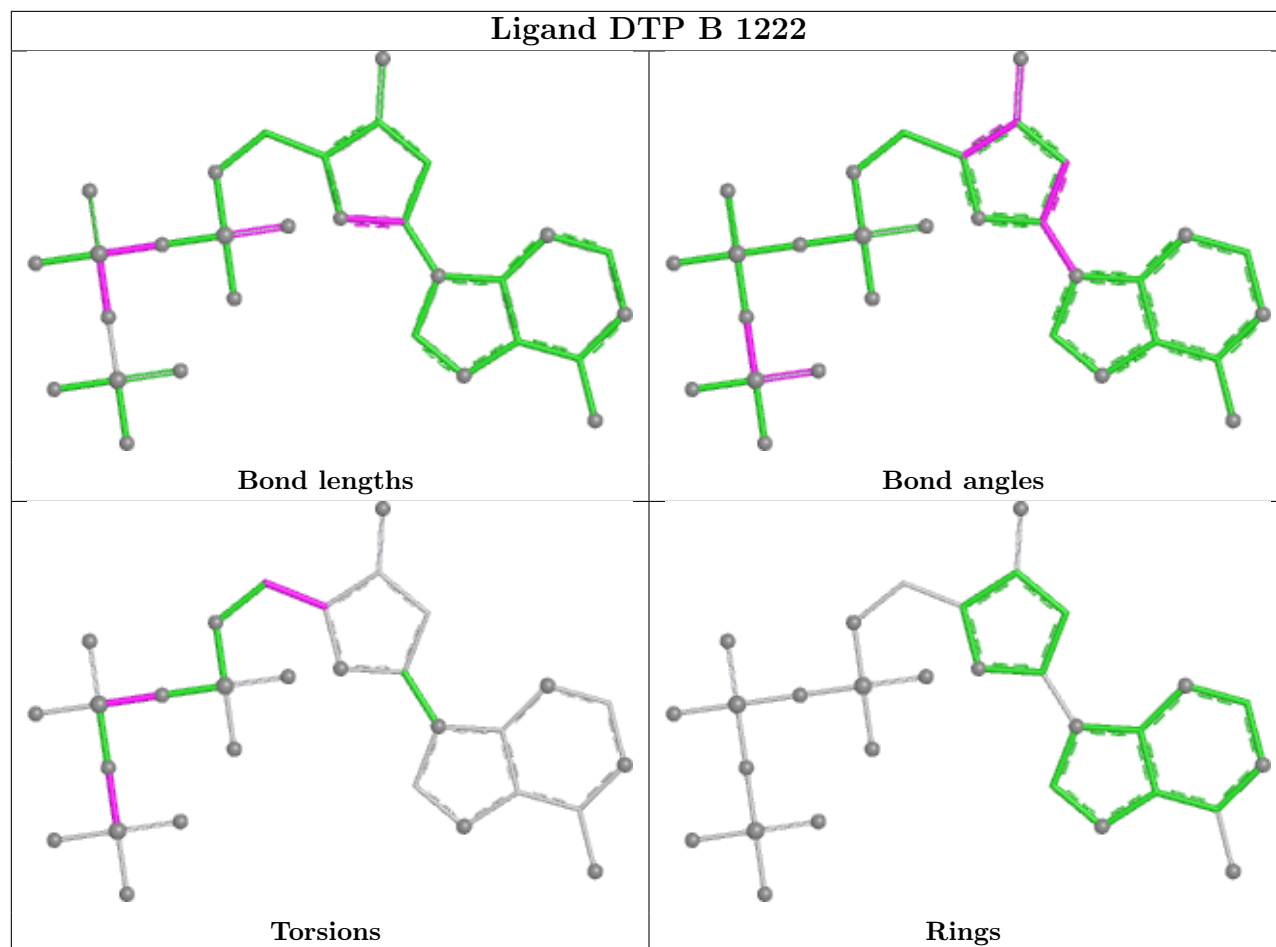
There are no ring outliers.

2 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1222	DTP	24	0
5	B	1222	DTP	14	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	12
3	A	9
1	C	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	575:HIS	C	576:ALA	N	3.18
1	B	575:HIS	C	576:ALA	N	3.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	812:GLY	C	813:PHE	N	2.78
1	B	812:GLY	C	813:PHE	N	2.56
1	B	285:LEU	C	286:PRO	N	2.49
1	A	491:GLN	C	492:ILE	N	2.48
1	B	567:GLY	C	568:LEU	N	2.42
1	C	24:DT	O3'	25:DT	P	2.13
1	B	699:PRO	C	700:GLY	N	2.06
1	A	567:GLY	C	568:LEU	N	1.99
1	D	3:DA	O3'	4:DA	P	1.96
1	B	713:HIS	C	714:GLY	N	1.94
1	B	491:GLN	C	492:ILE	N	1.88
1	B	397:MET	C	398:GLY	N	1.86
1	A	713:HIS	C	714:GLY	N	1.75
1	A	699:PRO	C	700:GLY	N	1.74
1	A	1127:ALA	C	1128:PRO	N	1.66
1	A	285:LEU	C	286:PRO	N	1.09
1	A	621:GLY	C	622:LEU	N	1.09
1	B	834:HIS	C	835:TYR	N	1.02
1	B	621:GLY	C	622:LEU	N	0.96
1	B	1127:ALA	C	1128:PRO	N	0.95
1	B	1026:SER	C	1027:CYS	N	0.89

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	C	20/27 (74%)	-0.45	0 100 100	228, 228, 228, 228	0
1	E	20/27 (74%)	-0.53	0 100 100	228, 228, 228, 228	0
2	D	18/21 (85%)	-0.56	0 100 100	66, 228, 228, 228	0
2	F	18/21 (85%)	-0.43	0 100 100	228, 228, 228, 228	0
3	A	1148/1220 (94%)	-0.55	9 (0%) 82 68	201, 226, 296, 326	0
3	B	1148/1220 (94%)	-0.53	15 (1%) 75 60	201, 226, 296, 326	0
All	All	2372/2536 (93%)	-0.54	24 (1%) 79 64	66, 226, 296, 326	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	496	GLY	4.0
3	A	771	LYS	4.0
3	B	497	SER	3.5
3	B	1188	LEU	3.3
3	A	139	LEU	3.1
3	B	447	GLY	3.0
3	B	1187	GLY	3.0
3	B	487	ASP	3.0
3	B	1005	ALA	3.0
3	A	567	GLY	2.8
3	B	584	GLU	2.4
3	A	23	ALA	2.4
3	A	504	LEU	2.4
3	B	585	PRO	2.3
3	A	1187	GLY	2.3
3	B	594	ARG	2.2
3	B	569	ASN	2.2
3	B	1194	TYR	2.2
3	B	1191	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	1189	LEU	2.1
3	A	521	LEU	2.1
3	A	140	ILE	2.0
3	B	10	LEU	2.0
3	A	586	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	D	21	18/19	0.98	0.07	227,227,227,227	0
2	DOC	F	21	18/19	0.99	0.05	227,227,227,227	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

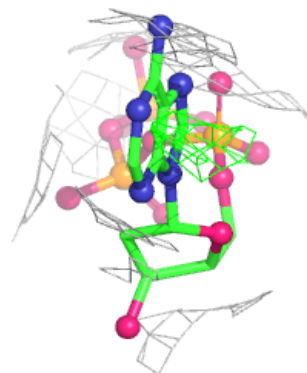
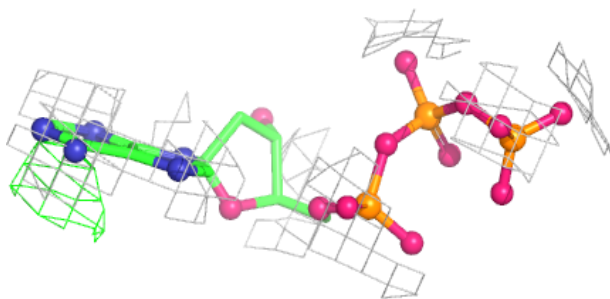
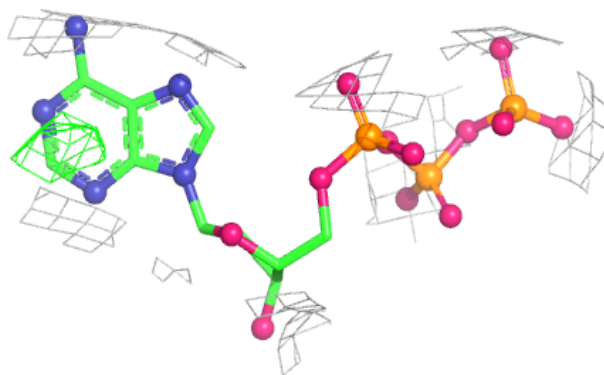
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DTP	A	1222	30/30	0.99	0.04	242,242,242,242	0
5	DTP	B	1222	30/30	0.99	0.05	242,242,242,242	0
4	CA	A	1221	1/1	1.00	0.01	47,47,47,47	0
4	CA	B	1221	1/1	1.00	0.01	47,47,47,47	0

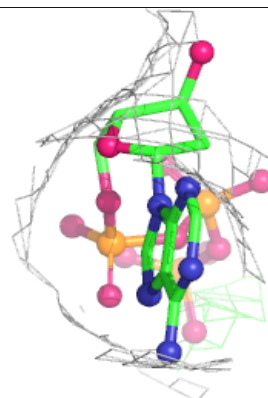
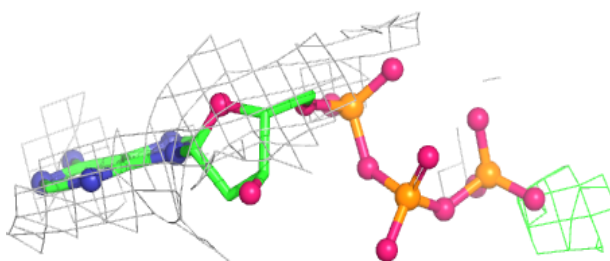
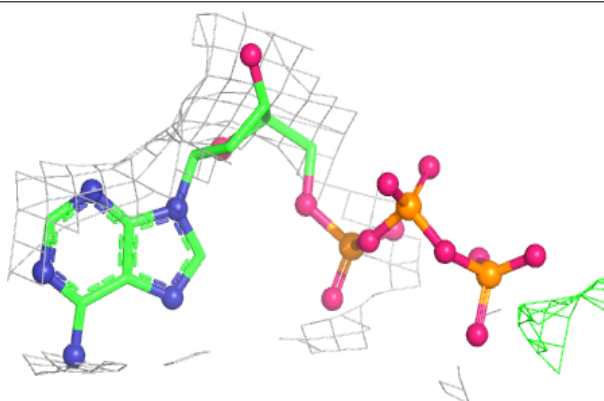
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP A 1222:

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

**Electron density around DTP B 1222:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.