Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 04:01 PM EDT

PDB ID	:	3E0D
Title	:	Insights into the Replisome from the Crystral 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 (i) symbol.

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

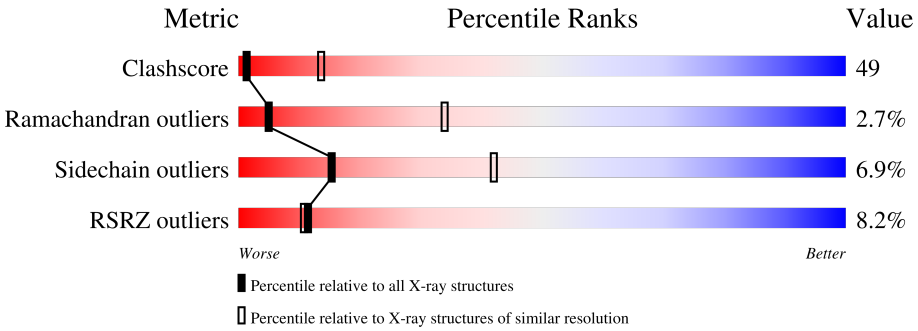
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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 <=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	4% · 67% · 26%
1	E	27	70% · 26%
2	D	21	5% 57% 24% 5% 10%
2	F	21	81% 10% 10%
3	A	1220	9% 61% 28% · · 6%
3	B	1220	7% 61% 28% · · 6%

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 (i)

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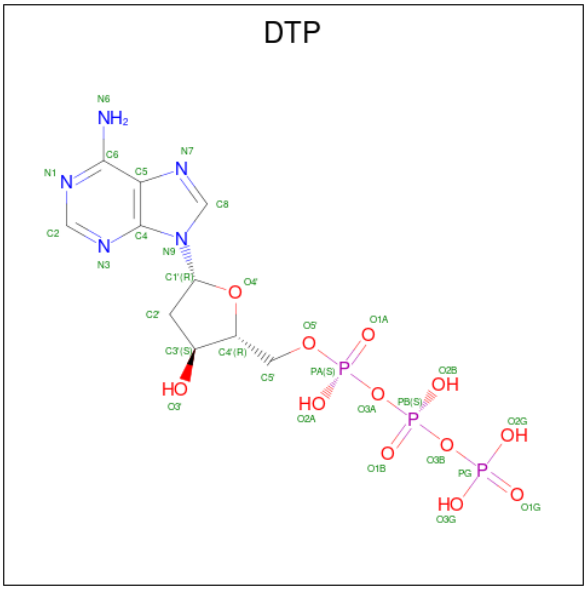
Chain	Residue	Modelled	Actual	Comment	Reference
B	539	PHE	ILE	engineered mutation	UNP Q9XDH5
B	540	GLU	GLN	engineered mutation	UNP Q9XDH5
B	541	ALA	VAL	engineered mutation	UNP Q9XDH5
B	542	GLU	VAL	engineered mutation	UNP Q9XDH5

- Molecule 4 is CALCIUM ION (three-letter code: 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 (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

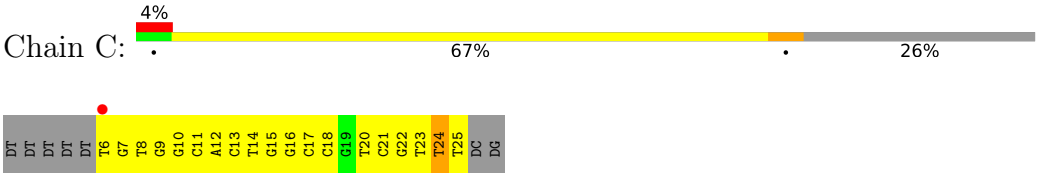


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 30 10 5 12 3	0	0
5	B	1	Total C N O P 30 10 5 12 3	0	0

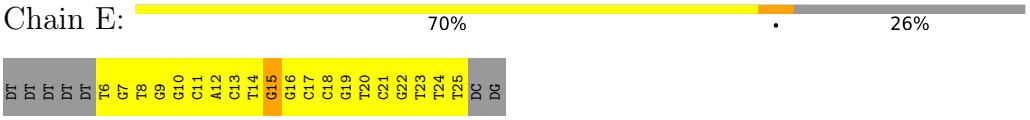
3 Residue-property plots (i)

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

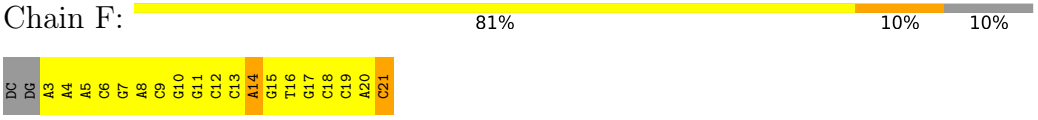


• Molecule 1: DNA substrate template strand

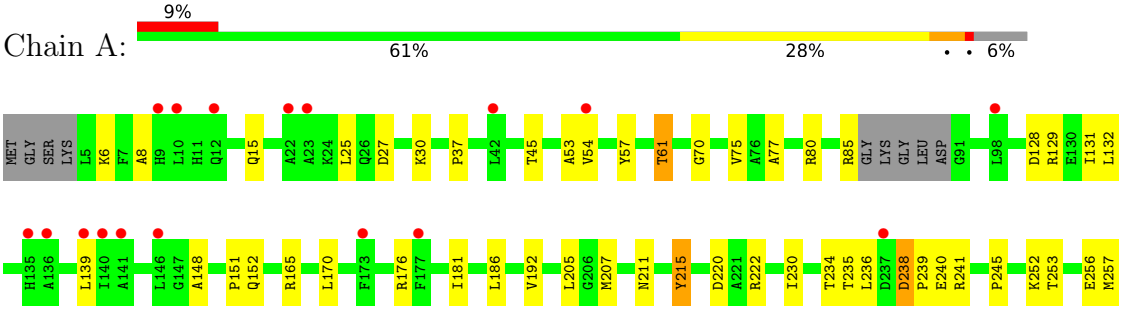


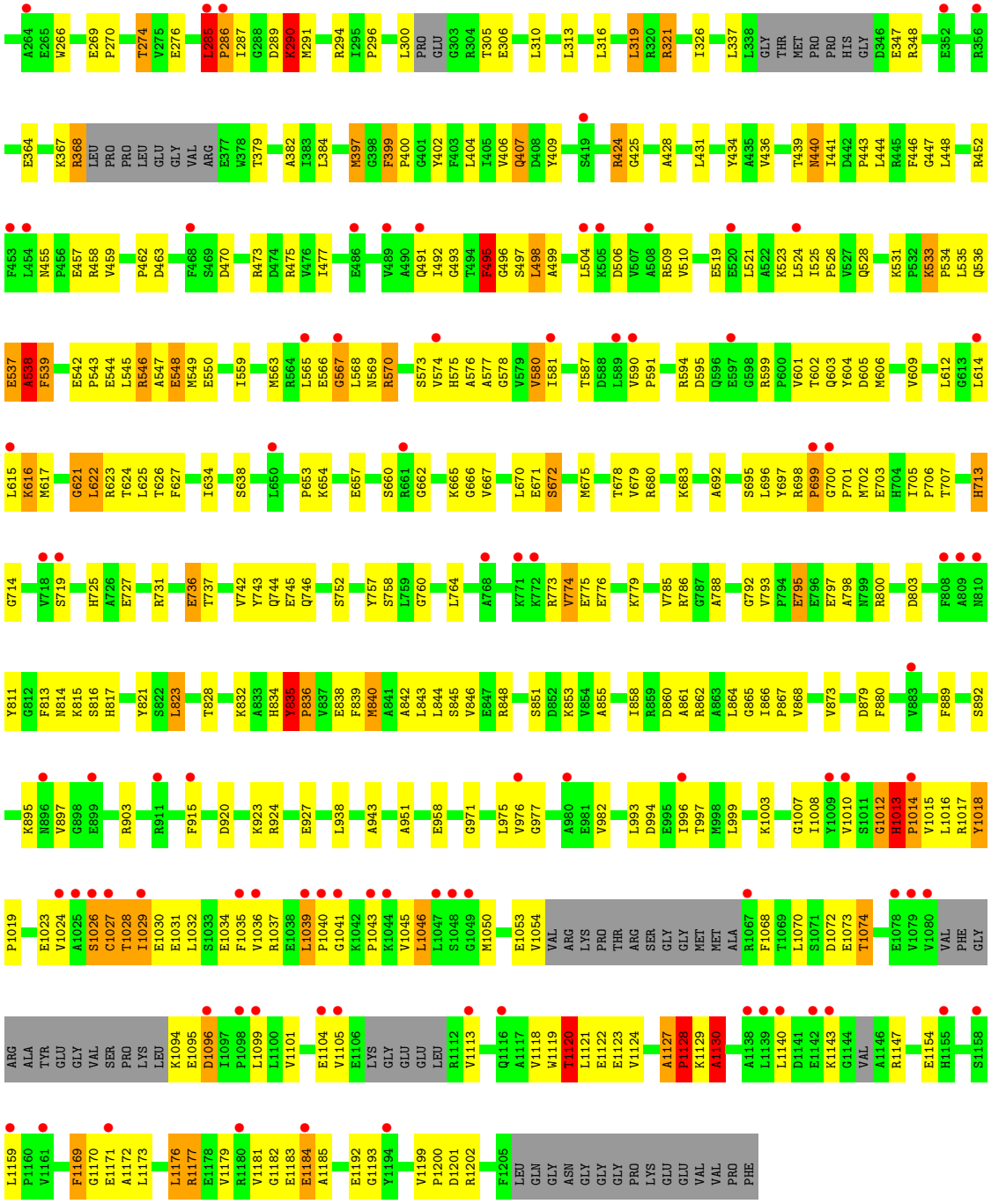
• Molecule 2: DNA substrate primer strand

• Molecule 2: DNA substrate primer strand



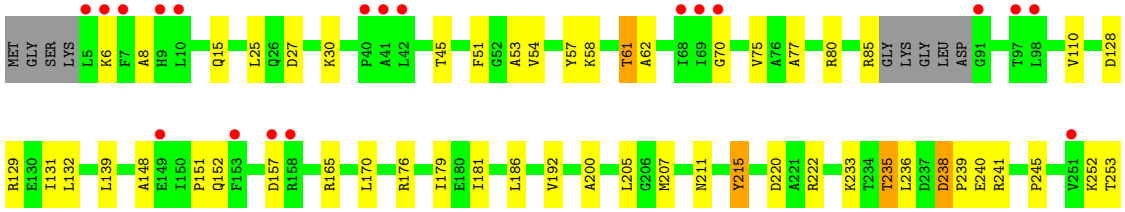
• Molecule 3: DNA polymerase III subunit alpha

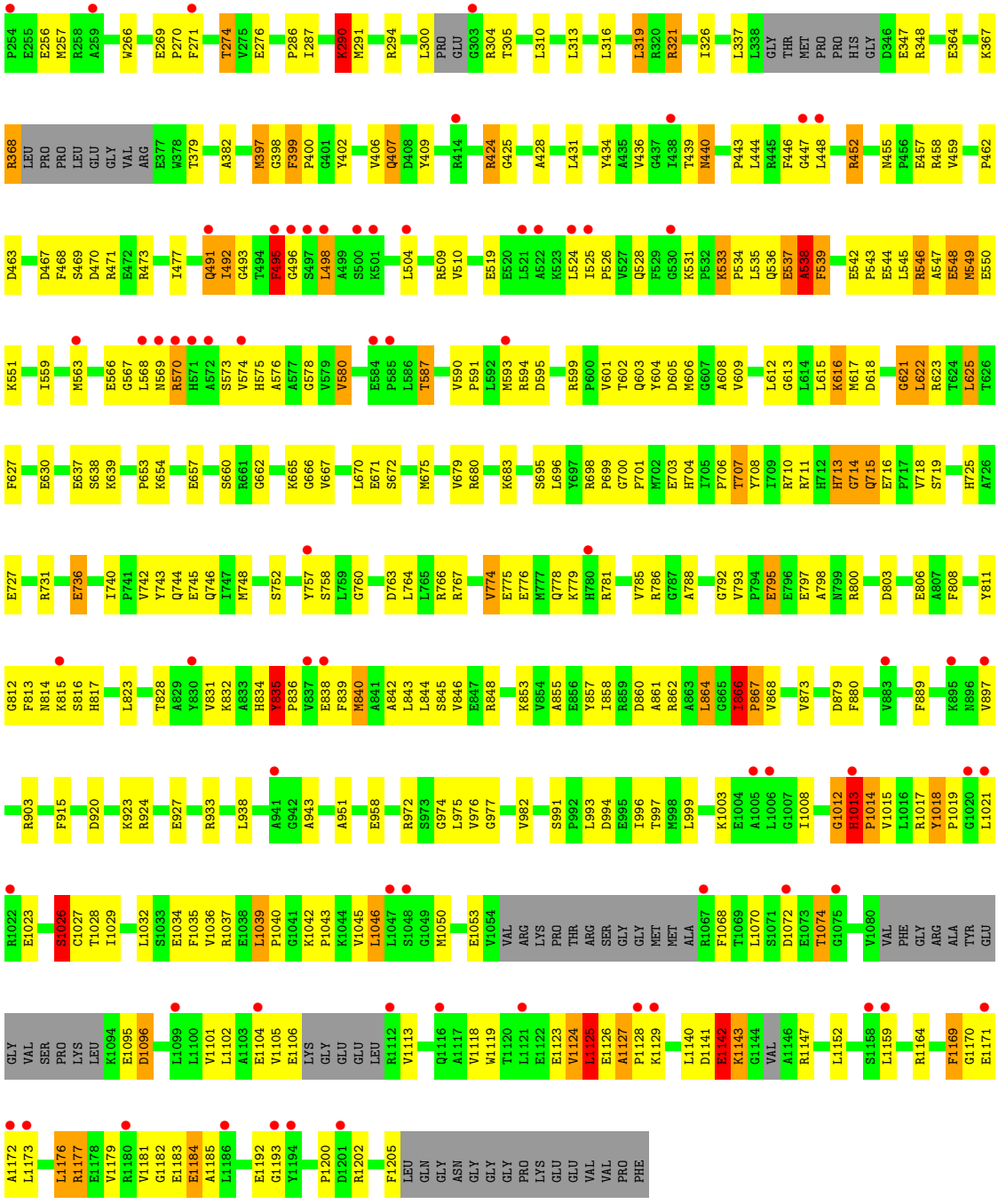




• Molecule 3: DNA polymerase III subunit alpha

Chain B:




P254 E255 E256 M257 R258 A259 W266 E269 P270 F271 T274 V275 E276 P286 I287 K290 M291 R294 L300 PRO GLU G303 R304 T305 L310 L313 L316 L319 R320 R321 I326 L337 L338 GLY THR MET PRO PRO HIS GLY D346 E347 R348 E364 K367
R368 LEU PRO PRO LEU GLU GLY VAL ARG E377 V378 T379 A382 M397 G398 F399 P400 G401 Y402 V406 Q407 D408 Y409 R414 R424 G425 A428 L431 Y434 A435 V436 G437 I438 T439 N440 P443 L444 R445 F446 G447 L448 R452 N455 P456 E457 R458 V459 P462
D463 D467 F468 S469 D470 R471 E472 R473 I477 Q491 I492 G493 T494 F496 G496 S497 L498 A499 S500 K501 L504 R509 V510 E519 E520 L521 A522 K523 L524 I525 P526 V527 Q528 F529 G530 K531 P532 K533 P534 L535 Q536 E537 A538 F539 E542 P543 E544 L545 R546 A547 E548 M549 E550
K551 I559 M563 E566 G567 L568 N569 R570 H571 A572 S573 V574 H575 A576 A577 G578 V579 V580 E584 P585 L586 T587 V590 P591 L592 M593 R594 D595 R599 P600 V601 T602 Q603 Y604 D605 M606 G607 A608 V609 L612 G613 L614 L615 K616 M617 D618 G621 L622 R623 T624 L625 T626
F627 E630 E637 S638 K639 P653 K654 E657 S660 R661 G662 K665 G666 V667 L670 E671 S672 M675 V679 R680 K683 S695 L696 Y697 R698 P699 G700 P701 M702 E703 H704 I705 P706 T707 Y708 I709 R710 R711 H712 H713 G714 Q715 E716 P717 V718 S719 H725 A726
E727 R731 E736 I740 P741 V742 Y743 Q744 E745 Q746 I747 W748 S752 Y757 S758 L759 G760 D763 L764 L765 R766 R767 V774 E775 E776 W777 Q778 K779 H780 R781 V785 R786 G787 A788 G792 V793 P794 E795 E796 E797 A798 N799 R800 D803 E806 A807 F808 Y811
G812 F813 N814 K815 S816 H817 L823 T828 A829 Y830 V831 K832 A833 H834 Y835 P836 V837 E838 F839 M840 A841 A842 L843 L844 S845 V846 E847 R848 K853 V854 A855 E856 Y857 I858 R859 D860 A861 R862 A863 L864 G865 T866 P867 V868 V873 D879 F880 V883 F889 K895 N896 V897
R903 F915 D920 K923 R924 E927 R933 L938 A941 G942 A943 A951 E958 R972 S973 G974 L975 V976 G977 V982 S991 P992 L993 D994 E995 I996 T997 M998 L999 K1003 E1004 A1005 L1006 G1007 I1008 G1012 H1013 P1014 V1015 L1016 R1017 Y1018 P1019 G1020 L1021
R1022 E1023 S1026 C1027 T1028 I1029 L1032 S1033 E1034 F1035 V1036 R1037 E1038 L1039 P1040 G1041 K1042 P1043 K1044 V1045 L1046 L1047 S1048 G1049 M1050 E1053 V1054 VAL ARG LYS PRO THR ARG SER GLY GLY MET MET ALA R1067 F1068 T1069 L1070 S1071 D1072 E1073 T1074 G1075 V1080 VAL PHE GLY ARG ALA TYR GLU
GLY VAL SER PRO LYS LEU K1094 E1095 D1096 L1099 L1100 V1101 L1102 A1103 E1104 V1105 E1106 LYS GLY GLU GLU LEU R1112 V1113 Q1116 A1117 V1118 W1119 T1120 L1121 E1122 E1123 V1124 L1125 E1126 A1127 P1128 K1129 L1140 D1141 E1142 K1143 G1144 VAL A1146 R1147 L1152 S1158 L1159 R1164 F1169 G1170 E1171
A1172 L1173 L1176 R1177 E1178 V1179 R1180 V1181 G1182 E1183 E1184 A1185 L1186 E1192 G1193 Y1194 P1200 D1201 R1202 F1205 LEU GLN GLY ASN GLY GLY GLY PRO LYS GLU GLU VAL VAL PRO PHE

4 Data and refinement statistics (i)

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 49.85 – 4.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.60) 99.5 (49.85-4.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 4.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.287 , 0.271 0.303 , (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)	0.28 , 198.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DTP, DOC, CA

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	2.18	1/454 (0.2%)	1.01	3/700 (0.4%)
1	E	0.74	1/454 (0.2%)	0.88	0/700
2	D	1.93	1/413 (0.2%)	1.24	6/635 (0.9%)
2	F	0.85	1/413 (0.2%)	0.95	0/635
3	A	0.68	13/9348 (0.1%)	1.00	21/12615 (0.2%)
3	B	0.79	14/9346 (0.1%)	0.84	20/12608 (0.2%)
All	All	0.84	31/20428 (0.2%)	0.94	50/27893 (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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	DT	O3'-P	43.89	2.13	1.61
3	B	713	HIS	C-N	34.20	1.94	1.33
3	B	397	MET	C-N	29.55	1.86	1.33
2	D	3	DA	O3'-P	29.28	1.96	1.61
3	A	567	GLY	C-N	28.47	1.99	1.34
3	B	491	GLN	C-N	23.63	1.88	1.34
3	A	713	HIS	C-N	23.63	1.75	1.33
3	A	699	PRO	C-N	22.99	1.74	1.33
3	B	1127	ALA	C-N	-20.20	0.95	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1026	SER	C-N	-19.57	0.89	1.34
3	A	1127	ALA	C-N	17.08	1.66	1.34
3	B	621	GLY	C-N	-16.52	0.96	1.34
3	B	834	HIS	C-N	-13.91	1.02	1.34
3	A	285	LEU	C-N	-13.02	1.09	1.34
3	A	621	GLY	C-N	-10.70	1.09	1.34
3	A	835	TYR	C-N	10.30	1.53	1.34
3	B	495	PHE	C-N	8.90	1.49	1.33
3	A	544	GLU	CD-OE2	8.04	1.34	1.25
3	B	544	GLU	CD-OE2	8.02	1.34	1.25
3	B	538	ALA	N-CA	7.54	1.61	1.46
3	A	538	ALA	N-CA	7.49	1.61	1.46
3	A	536	GLN	CG-CD	6.58	1.66	1.51
3	B	536	GLN	CG-CD	6.55	1.66	1.51
3	A	397	MET	C-N	6.35	1.44	1.33
2	F	14	DA	C5-C6	-6.11	1.35	1.41
3	B	538	ALA	CA-CB	-5.89	1.40	1.52
3	A	538	ALA	CA-CB	-5.88	1.40	1.52
3	B	835	TYR	C-N	-5.83	1.23	1.34
3	B	533	LYS	C-N	5.75	1.45	1.34
3	A	533	LYS	C-N	5.69	1.45	1.34
1	E	15	DG	C5-C6	-5.50	1.36	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	495	PHE	O-C-N	-47.05	43.21	123.20
3	A	699	PRO	CA-C-N	-41.86	32.49	116.20
3	A	699	PRO	C-N-CA	-39.91	38.49	122.30
3	A	1127	ALA	C-N-CD	-29.66	55.35	120.60
3	A	495	PHE	C-N-CA	-28.34	62.79	122.30
3	A	1127	ALA	O-C-N	-27.89	68.11	121.10
3	B	1127	ALA	CA-C-N	-26.69	42.36	117.10
3	A	495	PHE	CA-C-N	-24.46	67.27	116.20
3	A	835	TYR	CA-C-N	-19.41	62.77	117.10
3	A	835	TYR	C-N-CA	-19.13	41.67	122.00
3	A	495	PHE	O-C-N	-17.16	94.03	123.20
3	A	699	PRO	O-C-N	16.70	151.59	123.20
3	B	1127	ALA	C-N-CA	-15.28	57.84	122.00
3	B	1013	HIS	C-N-CD	-14.69	88.28	120.60
3	B	1127	ALA	C-N-CD	14.46	158.78	128.40
3	B	834	HIS	O-C-N	-12.76	102.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	DT	P-O3'-C3'	-12.36	104.86	119.70
3	A	397	MET	O-C-N	12.17	143.89	123.20
3	B	835	TYR	CA-C-N	-12.09	83.24	117.10
3	B	491	GLN	O-C-N	-11.90	103.66	122.70
3	A	1127	ALA	CA-C-N	11.53	149.37	117.10
3	B	835	TYR	C-N-CA	-11.03	75.68	122.00
3	B	1026	SER	O-C-N	-10.63	105.70	122.70
3	A	397	MET	CA-C-N	-10.63	94.95	116.20
3	B	495	PHE	C-N-CA	-10.60	100.05	122.30
3	A	397	MET	C-N-CA	-9.46	102.44	122.30
2	D	3	DA	P-O3'-C3'	9.14	130.67	119.70
3	B	834	HIS	CA-C-N	9.09	137.20	117.20
3	A	1013	HIS	C-N-CD	-8.71	101.44	120.60
3	A	567	GLY	O-C-N	-8.62	108.92	122.70
2	D	6	DC	OP1-P-O3'	8.57	124.06	105.20
3	B	835	TYR	C-N-CD	8.12	145.45	128.40
1	C	24	DT	OP2-P-O3'	7.96	122.71	105.20
3	A	835	TYR	O-C-N	-7.37	107.09	121.10
3	B	491	GLN	C-N-CA	-7.33	103.36	121.70
3	B	834	HIS	C-N-CA	7.20	139.70	121.70
3	B	491	GLN	CA-C-N	-6.86	102.11	117.20
3	A	285	LEU	CA-C-N	-6.85	97.92	117.10
3	A	567	GLY	C-N-CA	-6.68	105.00	121.70
3	A	621	GLY	O-C-N	-6.38	112.49	122.70
3	A	1127	ALA	C-N-CA	6.13	147.76	122.00
2	D	3	DA	OP1-P-O3'	6.13	118.69	105.20
3	B	397	MET	C-N-CA	5.73	134.33	122.30
2	D	7	DG	O5'-P-OP1	-5.71	100.56	105.70
3	B	1026	SER	CA-C-N	-5.70	104.66	117.20
2	D	4	DA	OP1-P-O3'	5.58	117.48	105.20
3	B	397	MET	O-C-N	-5.48	113.88	123.20
3	B	1127	ALA	O-C-N	5.32	131.21	121.10
2	D	3	DA	O3'-P-O5'	-5.07	94.37	104.00
1	C	24	DT	OP1-P-O3'	-5.02	94.16	105.20

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

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Mol	Chain	Res	Type	Atom
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	Peptide,Mainchain
3	B	864	LEU	Peptide
3	B	866	ILE	Peptide
2	D	11	DG	Sidechain
2	D	20	DA	Sidechain
2	D	7	DG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9168	0	9186	856	33
3	B	9168	0	9182	793	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	1892	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 (1892) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:713:HIS:C	3:A:714:GLY:N	1.75	1.40
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
3:A:458:ARG:NH1	3:A:764:LEU:CD2	1.92	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
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:B:397:MET:C	3:B:398:GLY:N	1.86	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:491:GLN:C	3:B:492:ILE:N	1.88	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
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
1:C:8:DT:H4'	3:A:622:LEU:CA	1.70	1.20
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: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
3:B:713:HIS:C	3:B:714:GLY:N	1.94	1.19
3:B:699:PRO:C	3:B:700:GLY:HA3	1.63	1.19
1:E:18:DC:OP1	3:B:933:ARG:HB2	1.40	1.19
3:A:845:SER:OG	3:A:879:ASP:OD2	1.59	1.18
3:A:775:GLU:OE1	3:B:781:ARG:NE	1.74	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:54:VAL:CG2	3:B:604:TYR:CZ	2.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:774:VAL:N	3:B:778:GLN:CD	1.74	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
3:A:773:ARG:HG2	3:B:778:GLN:CD	1.66	1.15
2:D:21:DOC:C2'	3:A:424:ARG:NH1	2.08	1.15
3:A:567:GLY:C	3:A:568:LEU:N	1.99	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
3:A:455:ASN:HD21	3:A:760:GLY:C	1.47	1.14
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: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:744:GLN:H	3:B:813:PHE:C	1.51	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:B:699:PRO:C	3:B:700:GLY:CA	2.15	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
3:A:523:LYS:CD	3:A:1094:LYS:HZ3	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:455:ASN:HD21	3:B:760:GLY:C	1.50	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: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: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:699:PRO:C	3:B:701:PRO:HD2	1.73	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
3:A:574:VAL:HG22	3:A:601:VAL:HG21	1.18	1.09
3:A:1129:LYS:HA	3:A:1199:VAL:C	1.71	1.09
3:B:699:PRO:C	3:B:700:GLY:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:812:GLY:C	3:B:813:PHE:HA	1.74	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: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
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
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
1:E:13:DC:C2'	1:E:14:DT:H5"	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1129:LYS:C	3:A:1199:VAL:O	1.99	1.00
3:A:774:VAL:HB	3:B:778:GLN:HG2	1.04	1.00
3:A:1028:THR:O	3:A:1031:GLU:N	1.93	1.00
3:B:743:TYR:C	3:B:813:PHE:N	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:1035:PHE:CE1	3:B:1171:GLU:C	2.37	0.98
2:D:21:DOC:H6	2:D:21:DOC:C5'	1.93	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
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:773:ARG:C	3:B:778:GLN:NE2	2.00	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:812:GLY:C	3:B:813:PHE:CA	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:779:LYS:HZ2	3:B:774:VAL:HA	1.33	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: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:773:ARG:CG	3:B:778:GLN:CD	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:GLY:H	3:B:815:LYS:HZ2	0.95	0.91
3:B:996:ILE:CD1	3:B:1017:ARG:HB3	1.99	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
3:B:866:ILE:HG22	3:B:867:PRO:C	1.92	0.91
3:A:1099:LEU:HD22	3:A:1119:TRP:O	1.71	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:775:GLU:CD	3:B:781:ARG:HE	1.74	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:A:698:ARG:C	3:A:701:PRO:HD2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:848:ARG:HE	3:B:879:ASP:CG	1.79	0.85
3:A:774:VAL:CG2	3:B:778:GLN:HG2	2.06	0.85
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:546:ARG:HD3	3:B:546:ARG:C	1.95	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
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:A:774:VAL:HG23	3:B:778:GLN:CG	2.07	0.83
3:B:447:GLY:N	3:B:815:LYS:HZ2	1.75	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: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
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
3:B:840:MET:HE2	3:B:840:MET:HA	1.62	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:523:LYS:HD2	3:A:1094:LYS:HZ2	1.42	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
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
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:743:TYR:C	3:A:813:PHE:N	2.34	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:845:SER:HG	3:A:879:ASP:CG	1.82	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:779:LYS:HZ1	3:B:774:VAL:HA	1.47	0.80
3:A:1013:HIS:ND1	3:A:1073:GLU:HB2	1.95	0.80
3:A:575:HIS:HD2	3:A:577:ALA:C	1.85	0.80
3:A:866:ILE:HG22	3:A:867:PRO:N	1.96	0.80
3:B:1125:LEU:O	3:B:1126:GLU:CG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:523:LYS:NZ	3:A:1054:VAL:HG22	1.97	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:699:PRO:C	3:B:701:PRO:CD	2.51	0.79
2:F:9:DC:H2"	2:F:10:DG:OP2	1.82	0.79
3:B:1123:GLU:O	3:B:1126:GLU:CD	2.21	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:523:LYS:HZ1	3:A:1054:VAL:HG22	1.48	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:A:840:MET:HE2	3:A:840:MET:HA	1.64	0.78
3:B:546:ARG:CD	3:B:546:ARG:C	2.51	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:B:8:ALA:H	3:B:274:THR:HG21	1.49	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:844:LEU:CG	3:A:880:PHE:CE1	2.68	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:LYS:HD2	3:A:1094:LYS:HZ1	1.43	0.77
2:F:18:DC:H2"	2:F:19:DC:OP2	1.83	0.77
3:A:546:ARG:CD	3:A:546:ARG:C	2.52	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:B:665:LYS:HD3	3:B:860:ASP:CG	2.04	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
3:A:745:GLU:CD	3:A:814:ASN:HA	2.06	0.77
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:546:ARG:C	3:A:546:ARG:HD3	2.05	0.76
3:A:1099:LEU:CD2	3:A:1119:TRP:O	2.33	0.76
3:B:665:LYS:CD	3:B:860:ASP:CG	2.50	0.76
3:A:745:GLU:OE1	3:A:814:ASN:HA	1.86	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:455:ASN:CG	3:A:760:GLY:CA	2.53	0.75
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:698:ARG:CG	3:A:701:PRO:CG	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:627:PHE:HE1	3:B:842:ALA:C	1.90	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
3:A:1034:GLU:CD	3:A:1170:GLY:HA2	2.07	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
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:775:GLU:CD	3:B:781:ARG:HH21	1.90	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:A:230:ILE:HD12	3:A:565:LEU:HD11	1.69	0.74
3:A:665:LYS:HD3	3:A:860:ASP:CG	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:455:ASN:CG	3:A:760:GLY:HA3	2.08	0.73
3:A:845:SER:OG	3:A:879:ASP:CG	2.26	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: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
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: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:B:567:GLY:C	3:B:568:LEU:N	2.42	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:523:LYS:HD3	3:A:1094:LYS:HZ3	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:627:PHE:HB2	3:A:846:VAL:HG21	1.70	0.71
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: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
3:A:699:PRO:C	3:A:701:PRO:CD	2.57	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
3:B:491:GLN:C	3:B:492:ILE:O	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:844:LEU:CD2	3:B:880:PHE:CE1	2.72	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:1140:LEU:HD12	3:B:1143:LYS:HZ1	1.54	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
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:845:SER:HA	3:A:879:ASP:CG	2.12	0.69
3:B:58:LYS:HB3	3:B:287:ILE:HD11	1.74	0.69
3:A:458:ARG:NH2	3:A:764:LEU:CD1	2.56	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:845:SER:CB	3:A:879:ASP:CG	2.62	0.68
3:B:831:VAL:CG1	3:B:839:PHE:CE1	2.69	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:DA:H1'	2:D:15:DG:C8	2.29	0.68
3:A:457:GLU:OE2	3:A:758:SER:CB	2.42	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:491:GLN:C	3:B:492:ILE:C	2.53	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: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:B:491:GLN:CD	3:B:574:VAL:HG11	2.14	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:A:491:GLN:C	3:A:492:ILE:N	2.48	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:743:TYR:HA	3:B:813:PHE:CA	2.26	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
3:A:1019:PRO:O	3:A:1023:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:710:ARG:NH1	3:B:716:GLU:CD	2.45	0.66
2:D:5:DA:H1'	2:D:6:DC:O5'	1.95	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:A:779:LYS:HZ2	3:B:774:VAL:CA	2.08	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: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
3:A:776:GLU:OE1	3:B:775:GLU:CD	2.34	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
3:B:491:GLN:C	3:B:492:ILE:CA	2.64	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: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:A:665:LYS:CD	3:A:860:ASP:CG	2.66	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
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:699:PRO:C	3:A:811:TYR:CD2	2.70	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
3:B:845:SER:HA	3:B:879:ASP:CG	2.18	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
3:B:1035:PHE:HE1	3:B:1171:GLU:C	1.97	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:A:575:HIS:CD2	3:A:577:ALA:C	2.67	0.63
3:A:745:GLU:CD	3:A:815:LYS:H	2.02	0.63
3:B:698:ARG:O	3:B:701:PRO:CD	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:699:PRO:C	3:A:701:PRO:HD2	2.17	0.63
3:B:458:ARG:CZ	3:B:764:LEU:HD11	2.28	0.63
3:B:627:PHE:CE1	3:B:842:ALA:C	2.72	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
3:B:1140:LEU:HD12	3:B:1143:LYS:HZ2	1.63	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:A:1028:THR:O	3:A:1029:ILE:C	2.37	0.62
3:B:698:ARG:HG3	3:B:811:TYR:HB3	1.80	0.62
3:B:1140:LEU:HB2	3:B:1143:LYS:HZ2	1.62	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: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
3:B:538:ALA:C	3:B:539:PHE:CD1	2.74	0.61
3:B:666:GLY:HA3	3:B:843:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:831:VAL:C	3:B:839:PHE:CD1	2.73	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: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:447:GLY:N	3:B:815:LYS:NZ	2.40	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:B:665:LYS:HB2	3:B:832:LYS:HZ1	1.65	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: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:1039:LEU:HB3	3:A:1040:PRO:HD2	1.82	0.61
3:B:535:LEU:HB3	3:B:563:MET:CE	2.31	0.61
1:C:12:DA:H1'	1:C:13:DC:C5'	2.31	0.60
3:A:538:ALA:C	3:A:539:PHE:CD1	2.74	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
2:D:20:DA:H4'	3:A:606:MET:HG3	1.82	0.60
3:A:627:PHE:HE1	3:A:842:ALA:C	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:547:ALA:C	3:A:549:MET:N	2.52	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:B:999:LEU:HD21	3:B:1012:GLY:C	2.21	0.60
3:A:701:PRO:CD	3:A:811:TYR:HB3	2.28	0.60
3:B:495:PHE:HZ	3:B:603:GLN:O	1.85	0.60
3:B:548:GLU:O	3:B:549:MET:C	2.40	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:455:ASN:CG	3:A:760:GLY:HA2	2.20	0.60
3:A:535:LEU:HB3	3:A:563:MET:CE	2.31	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:A:775:GLU:CD	3:B:781:ARG:NH2	2.55	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:546:ARG:NE	3:B:547:ALA:CB	2.59	0.59
3:B:627:PHE:HB2	3:B:846:VAL:HG21	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:535:LEU:HB3	3:B:563:MET:HE1	1.85	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:B:812:GLY:C	3:B:813:PHE:N	2.56	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: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:455:ASN:CG	3:B:760:GLY:CA	2.70	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:A:627:PHE:CE1	3:A:842:ALA:C	2.76	0.58
3:A:699:PRO:C	3:A:811:TYR:CE2	2.77	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:A:665:LYS:HB2	3:A:832:LYS:HZ1	1.67	0.58
3:B:470:ASP:OD2	3:B:623:ARG:HA	2.03	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
2:F:13:DC:H1'	2:F:14:DA:C8	2.39	0.57
3:A:665:LYS:HZ3	3:A:864:LEU:HD13	1.68	0.57
3:B:448:LEU:HD13	3:B:816:SER:CA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:523:LYS:HZ3	3:A:1054:VAL:HG13	1.70	0.57
3:A:665:LYS:CG	3:A:860:ASP:CG	2.72	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:A:665:LYS:NZ	3:A:864:LEU:HD13	2.20	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: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: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
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:697:TYR:CZ	3:A:702:MET:HE1	2.40	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:455:ASN:CG	3:B:760:GLY:HA3	2.26	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:A:845:SER:CA	3:A:879:ASP:CG	2.73	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: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:812:GLY:C	3:B:813:PHE:CB	2.74	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:B:424:ARG:HD3	5:B:1222:DTP:H4'	1.85	0.55
3:B:1035:PHE:HD1	3:B:1170:GLY:C	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:1013:HIS:O	3:A:1014:PRO:C	2.45	0.55
3:B:538:ALA:C	3:B:539:PHE:HD1	2.10	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: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
3:B:471:ARG:HH12	3:B:630:GLU:CD	2.10	0.54
1:C:14:DT:O2	2:D:14:DA:C2	2.60	0.54
3:A:538:ALA:C	3:A:539:PHE:HD1	2.10	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: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:A:535:LEU:HB3	3:A:563:MET:HE1	1.89	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
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: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:397:MET:CE	3:A:459:VAL:HA	2.38	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: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
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
1:C:9:DG:H21	3:A:576:ALA:CB	2.21	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:238:ASP:HB3	3:A:239:PRO:C	2.29	0.53
3:A:775:GLU:CD	3:B:781:ARG:NE	2.45	0.53
2:D:18:DC:H3'	3:A:499:ALA:HB2	1.89	0.53
3:A:547:ALA:O	3:A:548:GLU:C	2.47	0.53
3:A:996:ILE:HD11	3:A:1018:TYR:OH	2.08	0.53
3:A:547:ALA:C	3:A:549:MET:H	2.13	0.52
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
3:B:999:LEU:CD2	3:B:1012:GLY:C	2.77	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: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: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:457:GLU:CD	3:A:758:SER:OG	2.47	0.52
3:A:627:PHE:CE1	3:A:843:LEU:HG	2.45	0.52
3:B:51:PHE:CE2	3:B:593:MET:SD	3.03	0.52
3:B:238:ASP:HB3	3:B:239:PRO:C	2.29	0.52
3:B:699:PRO:C	3:B:811:TYR:CE1	2.61	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
3:A:239:PRO:O	3:A:240:GLU:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:58:LYS:HZ1	3:B:608:ALA:HA	1.73	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:496:GLY:O	3:A:569:ASN:CG	2.48	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: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:567:GLY:C	3:A:568:LEU:CA	2.76	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
3:B:1125:LEU:O	3:B:1126:GLU:CD	2.48	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:A:498:LEU:HB2	3:A:568:LEU:C	2.30	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:A:397:MET:HE3	3:A:459:VAL:HA	1.93	0.51
3:B:80:ARG:N	3:B:128:ASP:OD1	2.44	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

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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:1012:GLY:HA2	3:A:1013:HIS:HB2	1.92	0.51
3:B:714:GLY:C	3:B:715:GLN:HG3	2.24	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:257:MET:HE2	3:A:257:MET:HA	1.93	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
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
1:C:22:DG:C2	1:C:23:DT:C2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:812:GLY:C	3:B:813:PHE:HD1	2.15	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:9:DG:P	3:A:621:GLY:C	2.87	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
3:B:547:ALA:O	3:B:548:GLU:C	2.49	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:A:700:GLY:HA3	3:A:811:TYR:CD2	2.42	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:851:SER:CB	3:A:895:LYS:HZ3	2.23	0.49
3:B:832:LYS:HE3	3:B:840:MET:HE1	1.93	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:B:319:LEU:HD13	3:B:347:GLU:HG3	1.95	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:8:DT:O3'	3:A:622:LEU:C	2.50	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: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:1034:GLU:CD	3:A:1170:GLY:CA	2.80	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:A:848:ARG:HE	3:A:879:ASP:CG	2.16	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
1:C:9:DG:OP1	3:A:621:GLY:C	2.52	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:B:696:LEU:HG	3:B:742:VAL:CG1	2.43	0.48
3:A:321:ARG:NH2	3:A:440:ASN:ND2	2.42	0.48
3:B:812:GLY:C	3:B:813:PHE:CD1	2.87	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
3:B:1029:ILE:HG12	3:B:1072:ASP:CG	2.33	0.48
2:D:19:DC:C2'	3:A:531:LYS:HZ1	2.26	0.48
3:B:58:LYS:HZ3	3:B:608:ALA:HA	1.78	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
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: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: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:535:LEU:HB3	3:A:563:MET:HE2	1.96	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:665:LYS:CB	3:A:860:ASP:CG	2.78	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:548:GLU:C	3:B:550:GLU:N	2.69	0.46
3:B:696:LEU:HD11	3:B:742:VAL:CG2	2.45	0.46
3:B:848:ARG:NE	3:B:879:ASP:CG	2.53	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
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:A:744:GLN:H	3:A:813:PHE:C	2.19	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
3:B:1124:VAL:O	3:B:1125:LEU:C	2.54	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
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
3:B:236:LEU:O	3:B:241:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:397:MET:HE3	3:B:459:VAL:HA	1.98	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: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:A:1129:LYS:CA	3:A:1199:VAL:C	2.59	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:B:838:GLU:H	3:B:838:GLU:CD	2.20	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: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:A:838:GLU:CD	3:A:838:GLU:H	2.21	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:A:1121:LEU:C	3:A:1123:GLU:N	2.69	0.44
3:B:468:PHE:C	3:B:625:LEU:HD23	2.37	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: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: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:575:HIS:NE2	3:A:577:ALA:HB3	2.33	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: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:A:775:GLU:CD	3:B:781:ARG:CZ	2.86	0.43
3:B:402:TYR:CE1	3:B:615:LEU:CD1	3.01	0.43
3:B:535:LEU:HB3	3:B:563:MET:HE2	2.00	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: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:234:THR:C	3:A:510:VAL:HG13	2.36	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:310:LEU:CD2	3:A:400:PRO:HA	2.48	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: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
3:B:1142:GLU:C	3:B:1143:LYS:HG3	2.40	0.42
1:E:10:DG:C2'	1:E:11:DC:C5	3.01	0.42
3:A:1028:THR:C	3:A:1030:GLU:N	2.71	0.42
3:B:252:LYS:HD2	3:B:257:MET:HE2	2.01	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:773:ARG:HG2	3:B:778:GLN:CG	2.46	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:A:252:LYS:HD2	3:A:257:MET:CE	2.50	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
1:C:14:DT:H2"	1:C:15:DG:O5'	2.19	0.42
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:1034:GLU:CG	3:A:1170:GLY:CA	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:525:ILE:HA	3:B:526:PRO:HD3	1.90	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: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:1036:VAL:O	3:B:1037:ARG:C	2.58	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: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:A:1036:VAL:O	3:A:1037:ARG:C	2.58	0.42
3:B:257:MET:HE2	3:B:257:MET:HA	2.00	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: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
3:B:744:GLN:HG3	3:B:813:PHE:C	2.41	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1072:ASP:C	3:B:1074:THR:H	2.23	0.41
3:A:257:MET:HA	3:A:257:MET:CE	2.50	0.41
3:A:316:LEU:HD21	3:A:348:ARG:HA	2.02	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
3:B:1182:GLY:O	3:B:1183:GLU:HB2	2.21	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:321:ARG:CG	3:B:434:TYR:CE2	3.03	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
2:F:20:DA:C3'	2:F:21:DOC:H5'	2.47	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
3:A:1072:ASP:C	3:A:1074:THR:H	2.23	0.41
3:B:1035:PHE:CD1	3:B:1171:GLU:C	2.89	0.41
1:C:9:DG:OP1	3:A:621:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:779:LYS:HZ2	3:B:774:VAL:HG13	1.86	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:B:27:ASP:HA	3:B:30:LYS:HG2	2.03	0.41
3:B:257:MET:HA	3:B:257:MET:CE	2.50	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:523:LYS:HZ3	3:A:1054:VAL:HG22	1.80	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
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:665:LYS:CD	3:A:860:ASP:CB	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:470:ASP:CG	3:A:626:THR:HG1	2.25	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1124/1220 (92%)	1006 (90%)	88 (8%)	30 (3%)	5	34
3	B	1120/1220 (92%)	1007 (90%)	82 (7%)	31 (3%)	5	33
All	All	2244/2440 (92%)	2013 (90%)	170 (8%)	61 (3%)	5	34

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
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

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Mol	Chain	Res	Type
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)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	953/1008 (94%)	889 (93%)	64 (7%)	16	43
3	B	953/1008 (94%)	886 (93%)	67 (7%)	15	41
All	All	1906/2016 (94%)	1775 (93%)	131 (7%)	15	42

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	LYS
3	A	61	THR
3	A	75	VAL
3	A	85	ARG
3	A	132	LEU

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Mol	Chain	Res	Type
3	A	165	ARG
3	A	207	MET
3	A	211	ASN
3	A	215	TYR
3	A	222	ARG
3	A	235	THR
3	A	253	THR
3	A	274	THR
3	A	276	GLU
3	A	290	LYS
3	A	300	LEU
3	A	305	THR
3	A	319	LEU
3	A	321	ARG
3	A	326	ILE
3	A	368	ARG
3	A	407	GLN
3	A	424	ARG
3	A	439	THR
3	A	440	ASN
3	A	444	LEU
3	A	452	ARG
3	A	463	ASP
3	A	498	LEU
3	A	519	GLU
3	A	546	ARG
3	A	580	VAL
3	A	587	THR
3	A	616	LYS
3	A	617	MET
3	A	622	LEU
3	A	625	LEU
3	A	670	LEU
3	A	672	SER
3	A	707	THR
3	A	719	SER
3	A	736	GLU
3	A	786	ARG
3	A	795	GLU
3	A	823	LEU
3	A	840	MET
3	A	903	ARG

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Mol	Chain	Res	Type
3	A	927	GLU
3	A	958	GLU
3	A	997	THR
3	A	1018	TYR
3	A	1026	SER
3	A	1028	THR
3	A	1032	LEU
3	A	1045	VAL
3	A	1046	LEU
3	A	1074	THR
3	A	1095	GLU
3	A	1096	ASP
3	A	1104	GLU
3	A	1120	THR
3	A	1169	PHE
3	A	1184	GLU
3	A	1192	GLU
3	B	6	LYS
3	B	61	THR
3	B	75	VAL
3	B	85	ARG
3	B	132	LEU
3	B	165	ARG
3	B	207	MET
3	B	211	ASN
3	B	215	TYR
3	B	222	ARG
3	B	235	THR
3	B	253	THR
3	B	274	THR
3	B	276	GLU
3	B	290	LYS
3	B	300	LEU
3	B	305	THR
3	B	319	LEU
3	B	321	ARG
3	B	326	ILE
3	B	368	ARG
3	B	407	GLN
3	B	424	ARG
3	B	439	THR
3	B	440	ASN

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Mol	Chain	Res	Type
3	B	444	LEU
3	B	452	ARG
3	B	463	ASP
3	B	498	LEU
3	B	519	GLU
3	B	546	ARG
3	B	580	VAL
3	B	587	THR
3	B	616	LYS
3	B	617	MET
3	B	622	LEU
3	B	625	LEU
3	B	670	LEU
3	B	672	SER
3	B	707	THR
3	B	719	SER
3	B	736	GLU
3	B	786	ARG
3	B	795	GLU
3	B	823	LEU
3	B	840	MET
3	B	866	ILE
3	B	903	ARG
3	B	927	GLU
3	B	958	GLU
3	B	997	THR
3	B	1013	HIS
3	B	1018	TYR
3	B	1027	CYS
3	B	1028	THR
3	B	1032	LEU
3	B	1045	VAL
3	B	1046	LEU
3	B	1074	THR
3	B	1095	GLU
3	B	1096	ASP
3	B	1104	GLU
3	B	1125	LEU
3	B	1142	GLU
3	B	1169	PHE
3	B	1184	GLU
3	B	1192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	9	HIS
3	A	15	GLN
3	A	440	ASN
3	A	455	ASN
3	A	575	HIS
3	A	725	HIS
3	A	746	GLN
3	A	1013	HIS
3	A	1116	GLN
3	A	1155	HIS
3	B	9	HIS
3	B	15	GLN
3	B	440	ASN
3	B	455	ASN
3	B	569	ASN
3	B	575	HIS
3	B	725	HIS
3	B	746	GLN
3	B	778	GLN
3	B	817	HIS
3	B	1013	HIS
3	B	1116	GLN
3	B	1155	HIS

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	14,19,20	1.07	2 (14%)	13,26,29	1.38	2 (15%)
2	DOC	F	21	2,1	14,19,20	1.07	1 (7%)	13,26,29	1.37	1 (7%)

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	-	2/4/18/19	0/2/2/2
2	DOC	F	21	2,1	-	2/4/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	DOC	O5'-C5'	-2.22	1.39	1.44
2	D	21	DOC	C6-C5	-2.20	1.33	1.38
2	F	21	DOC	C6-C5	-2.13	1.33	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	21	DOC	C2-N3-C4	3.83	120.23	116.34
2	D	21	DOC	C2-N3-C4	3.80	120.19	116.34
2	D	21	DOC	C3'-C2'-C1'	2.32	105.45	102.78

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	26,32,32	1.27	2 (7%)	30,50,50	1.28	4 (13%)
5	DTP	B	1222	4	26,32,32	1.27	2 (7%)	30,50,50	1.28	4 (13%)

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	-	5/18/34/34	0/3/3/3
5	DTP	B	1222	4	-	5/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1222	DTP	O4'-C1'	-3.10	1.35	1.42
5	A	1222	DTP	O4'-C1'	-3.09	1.35	1.42
5	B	1222	DTP	PA-O2A	-2.69	1.42	1.55
5	A	1222	DTP	PA-O2A	-2.66	1.42	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1222	DTP	C2'-C1'-N9	-3.07	107.20	114.27
5	B	1222	DTP	C2'-C1'-N9	-3.03	107.28	114.27
5	B	1222	DTP	O3'-C3'-C4'	2.91	121.23	110.10
5	A	1222	DTP	O3'-C3'-C4'	2.89	121.17	110.10
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
5	B	1222	DTP	C5-C6-N6	2.07	123.50	120.35
5	A	1222	DTP	C5-C6-N6	2.01	123.40	120.35

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.

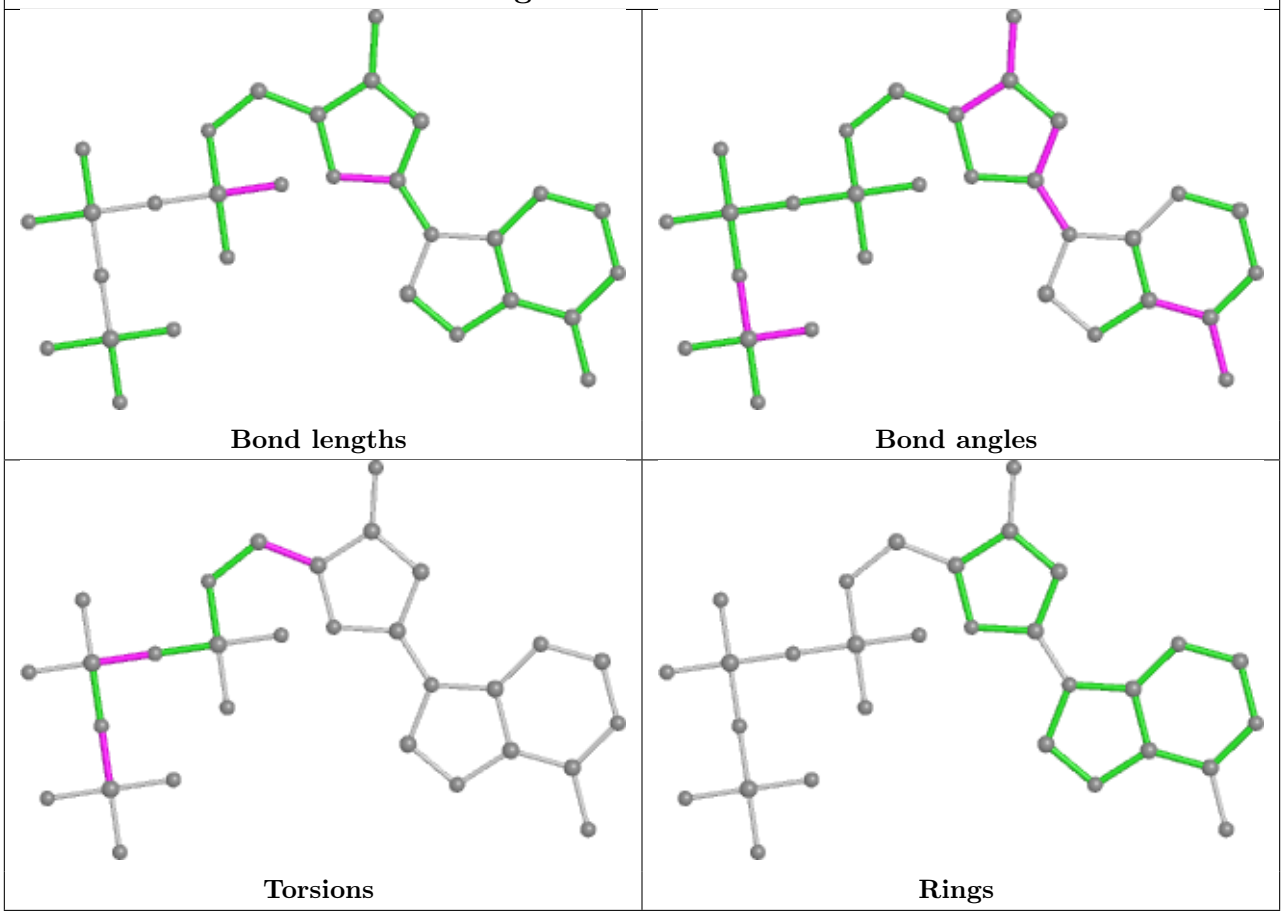
2 monomers are involved in 38 short contacts:

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

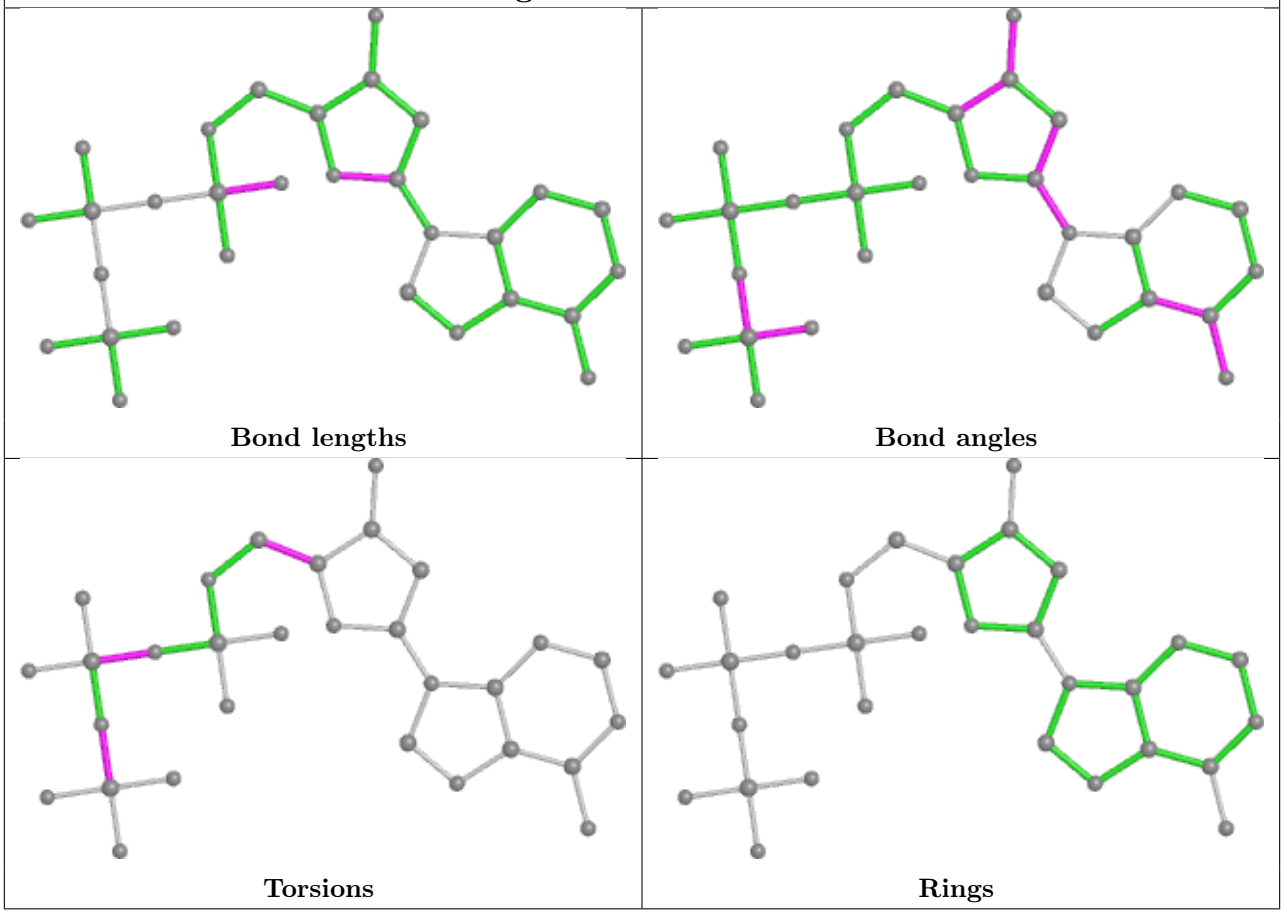
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand DTP A 1222



Ligand DTP B 1222



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	20/27 (74%)	-0.30	1 (5%) 28 25	228, 228, 228, 228	0
1	E	20/27 (74%)	-0.63	0 100 100	228, 228, 228, 228	0
2	D	18/21 (85%)	-0.50	0 100 100	66, 228, 228, 228	0
2	F	18/21 (85%)	-0.50	0 100 100	228, 228, 228, 228	0
3	A	1148/1220 (94%)	0.34	105 (9%) 9 8	201, 226, 296, 326	0
3	B	1148/1220 (94%)	0.33	88 (7%) 13 12	201, 226, 296, 326	0
All	All	2372/2536 (93%)	0.31	194 (8%) 11 11	66, 226, 296, 326	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1026	SER	8.0
3	B	496	GLY	7.8
3	B	569	ASN	7.2
3	B	1129	LYS	6.4
3	B	524	LEU	6.3
3	A	1049	GLY	6.0
3	B	5	LEU	6.0
3	A	23	ALA	5.9
3	B	525	ILE	5.8
3	A	1139	LEU	5.4
3	B	574	VAL	5.3
3	A	718	VAL	5.1
3	B	447	GLY	5.0
3	B	10	LEU	5.0
3	B	1172	ALA	5.0
3	A	139	LEU	4.9
3	A	141	ALA	4.8
3	B	6	LYS	4.8
3	A	1035	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
3	B	497	SER	4.7
3	A	1040	PRO	4.6
3	A	1138	ALA	4.6
3	A	140	ILE	4.5
3	B	1171	GLU	4.4
3	A	505	LYS	4.3
3	B	98	LEU	4.3
3	B	254	PRO	4.3
3	B	584	GLU	4.2
3	B	572	ALA	4.2
3	A	1180	ARG	4.2
3	A	1044	LYS	4.2
3	A	1027	CYS	4.2
3	B	1193	GLY	4.2
3	B	1048	SER	4.2
3	A	1098	PRO	4.1
3	B	97	THR	4.1
3	A	1140	LEU	4.1
3	A	22	ALA	4.1
3	B	495	PHE	4.0
3	B	1116	GLN	4.0
3	B	9	HIS	4.0
3	B	1201	ASP	3.9
3	B	1020	GLY	3.8
3	B	1194	TYR	3.8
3	B	149	GLU	3.7
3	A	1039	LEU	3.7
3	A	1096	ASP	3.7
3	A	1116	GLN	3.7
3	B	501	LYS	3.6
3	B	69	ILE	3.6
3	B	1180	ARG	3.6
3	B	1072	ASP	3.5
3	B	570	ARG	3.5
3	A	1048	SER	3.5
3	B	414	ARG	3.5
3	A	1041	GLY	3.5
3	B	7	PHE	3.4
3	B	1173	LEU	3.3
3	A	996	ILE	3.3
3	B	504	LEU	3.3
3	B	522	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	B	303	GLY	3.3
3	B	1005	ALA	3.3
3	B	41	ALA	3.2
3	B	1075	GLY	3.2
3	A	650	LEU	3.2
3	B	883	VAL	3.2
3	B	895	LYS	3.2
3	A	1158	SER	3.2
3	A	524	LEU	3.2
3	A	771	LYS	3.2
3	A	1159	LEU	3.1
3	B	1099	LEU	3.1
3	A	146	LEU	3.1
3	A	1113	VAL	3.1
3	A	1036	VAL	3.1
3	B	1128	PRO	3.1
3	A	615	LEU	3.1
3	B	1021	LEU	3.1
3	B	1013	HIS	3.1
3	B	1186	LEU	3.0
3	A	1099	LEU	3.0
3	A	1078	GLU	3.0
3	A	589	LEU	3.0
3	A	883	VAL	3.0
3	A	1079	VAL	3.0
3	A	1024	VAL	3.0
3	A	1184	GLU	3.0
3	B	838	GLU	3.0
3	A	10	LEU	3.0
3	A	1194	TYR	2.9
3	A	453	PHE	2.9
3	A	1080	VAL	2.8
3	B	1112	ARG	2.8
3	B	1121	LEU	2.8
3	A	1142	GLU	2.8
3	A	1025	ALA	2.8
3	B	157	ASP	2.8
3	B	815	LYS	2.8
3	B	42	LEU	2.7
3	B	941	ALA	2.7
3	A	135	HIS	2.7
3	B	521	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	42	LEU	2.7
3	A	264	ALA	2.7
3	A	1161	VAL	2.7
3	A	504	LEU	2.7
3	B	568	LEU	2.6
3	A	565	LEU	2.6
3	A	286	PRO	2.6
3	A	581	ILE	2.6
3	B	91	GLY	2.6
3	A	590	VAL	2.6
3	A	419	SER	2.6
3	B	500	SER	2.6
3	A	567	GLY	2.5
3	A	768	ALA	2.5
3	A	1143	LYS	2.5
3	A	810	ASN	2.5
3	A	486	GLU	2.5
3	A	1043	PRO	2.5
3	A	808	PHE	2.5
3	A	700	GLY	2.5
3	B	593	MET	2.5
3	B	1159	LEU	2.5
3	A	574	VAL	2.5
3	A	896	ASN	2.5
3	B	448	LEU	2.5
3	B	1067	ARG	2.5
3	B	563	MET	2.4
3	A	1105	VAL	2.4
3	A	1029	ILE	2.4
3	A	468	PHE	2.4
3	A	177	PHE	2.4
3	B	251	VAL	2.4
3	A	699	PRO	2.4
3	B	491	GLN	2.3
3	B	259	ALA	2.3
3	A	614	LEU	2.3
3	A	1014	PRO	2.3
3	A	911	ARG	2.3
3	A	489	VAL	2.3
3	B	1158	SER	2.3
3	A	1009	TYR	2.3
3	B	158	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	285	LEU	2.3
3	B	1047	LEU	2.3
3	A	719	SER	2.3
3	A	661	ARG	2.3
3	A	915	PHE	2.3
3	A	98	LEU	2.3
3	A	1155	HIS	2.2
3	A	899	GLU	2.2
3	B	897	VAL	2.2
3	B	571	HIS	2.2
3	A	520	GLU	2.2
3	B	530	GLY	2.2
3	A	9	HIS	2.2
3	A	597	GLU	2.2
1	C	6	DT	2.2
3	B	1104	GLU	2.2
3	A	491	GLN	2.2
3	B	438	ILE	2.2
3	B	498	LEU	2.2
3	A	237	ASP	2.2
3	A	809	ALA	2.1
3	B	830	TYR	2.1
3	A	976	VAL	2.1
3	A	54	VAL	2.1
3	A	454	LEU	2.1
3	A	136	ALA	2.1
3	B	40	PRO	2.1
3	A	1047	LEU	2.1
3	B	68	ILE	2.1
3	B	1006	LEU	2.1
3	A	1104	GLU	2.1
3	B	70	GLY	2.1
3	A	352	GLU	2.1
3	B	585	PRO	2.1
3	B	271	PHE	2.1
3	A	1067	ARG	2.0
3	A	356	ARG	2.0
3	A	12	GLN	2.0
3	A	508	ALA	2.0
3	B	757	TYR	2.0
3	A	1171	GLU	2.0
3	A	980	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	B	780	HIS	2.0
3	A	1010	VAL	2.0
3	B	837	VAL	2.0
3	A	772	LYS	2.0
3	B	1022	ARG	2.0
3	A	173	PHE	2.0
3	B	153	PHE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DOC	F	21	18/19	0.67	0.26	227,227,227,227	0
2	DOC	D	21	18/19	0.78	0.19	227,227,227,227	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

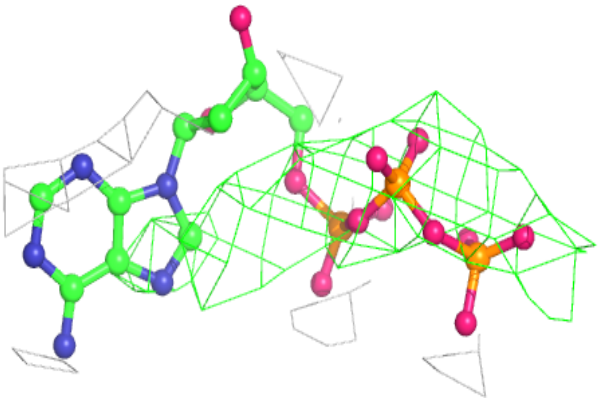
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

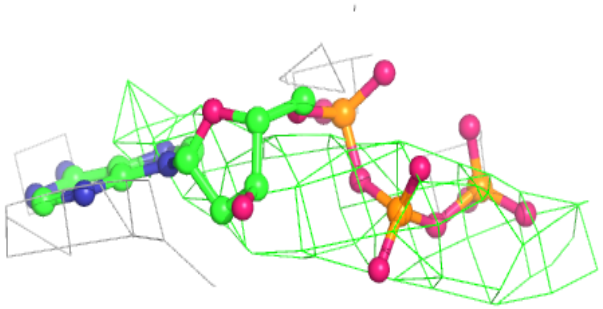
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DTP	B	1222	30/30	0.80	0.28	242,242,242,242	0
5	DTP	A	1222	30/30	0.83	0.25	242,242,242,242	0
4	CA	B	1221	1/1	0.96	0.24	47,47,47,47	0
4	CA	A	1221	1/1	0.97	0.26	47,47,47,47	0

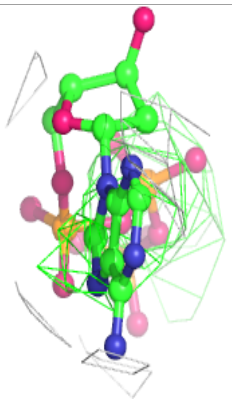
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP 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)

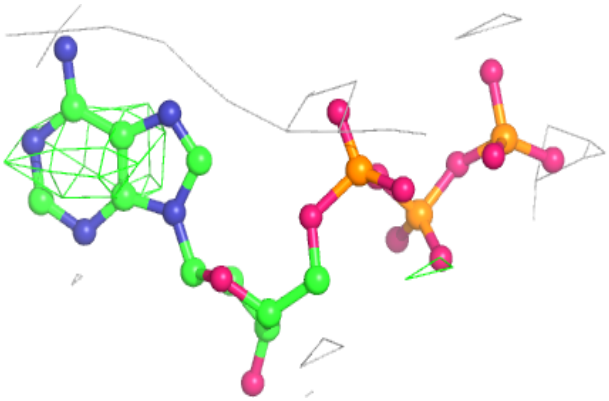


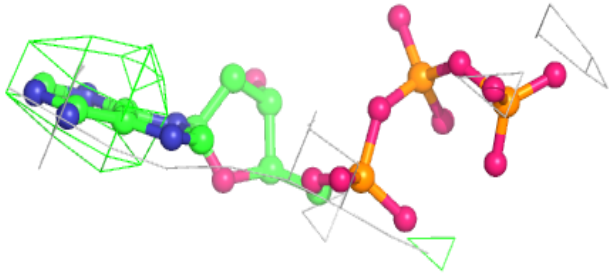


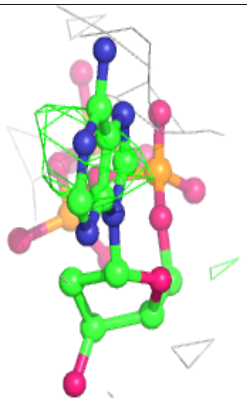


Electron density around DTP A 1222:

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







6.5 Other polymers (i)

There are no such residues in this entry.