



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:22 am BST

PDB ID : 2AGP
Title : Fidelity of Dpo4: effect of metal ions, nucleotide selection and pyrophosphorolysis
Authors : Ling, H.; Yang, W.
Deposited on : 2005-07-27
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

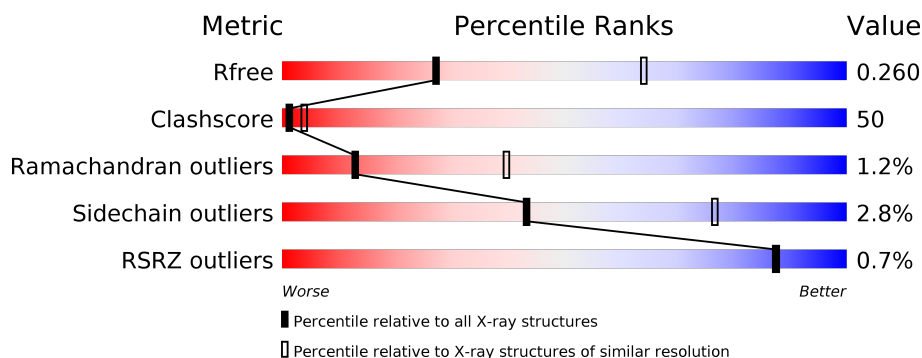
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	C	13	<div> <div>15%</div> <div>77%</div> <div>8%</div> </div>
1	E	13	<div> <div>8%</div> <div>92%</div> </div>
2	D	17	<div> <div>12%</div> <div>53%</div> <div>35%</div> </div>
2	F	17	<div> <div>6%</div> <div>82%</div> <div>6%</div> <div>6%</div> </div>
3	A	341	<div> <div>%</div> <div>47%</div> <div>50%</div> <div>.</div> </div>
3	B	341	<div> <div>50%</div> <div>48%</div> <div>.</div> </div>

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
1	DOC	C	1813	-	-	-	X
1	DOC	E	1813	-	-	X	-
6	DGT	A	401	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7506 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 (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	0	0	0
			272	129	57	74	12			
1	E	13	Total	C	N	O	P	0	0	0
			272	129	57	74	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	P	0	0	0
			334	163	50	105	16			
2	F	17	Total	C	N	O	P	0	0	0
			334	163	50	105	16			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2744	1760	472	505	7			
3	B	341	Total	C	N	O	S	0	0	0
			2744	1760	472	505	7			

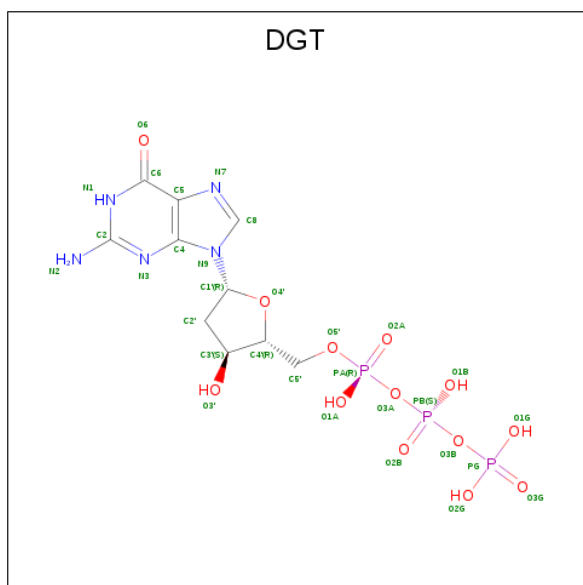
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Mg 3 3	0	0
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	57	Total O 57 57	0	0
7	D	49	Total O 49 49	0	0
7	E	38	Total O 38 38	0	0
7	F	56	Total O 56 56	0	0
7	A	257	Total O 257 257	0	0

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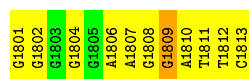
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	280	Total 280	O 280	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

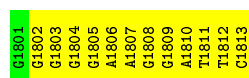
- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC)-3')

Chain C: 




- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC)-3')

Chain E: 



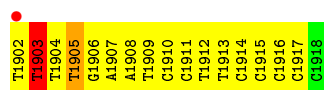
- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3')

Chain D: 



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

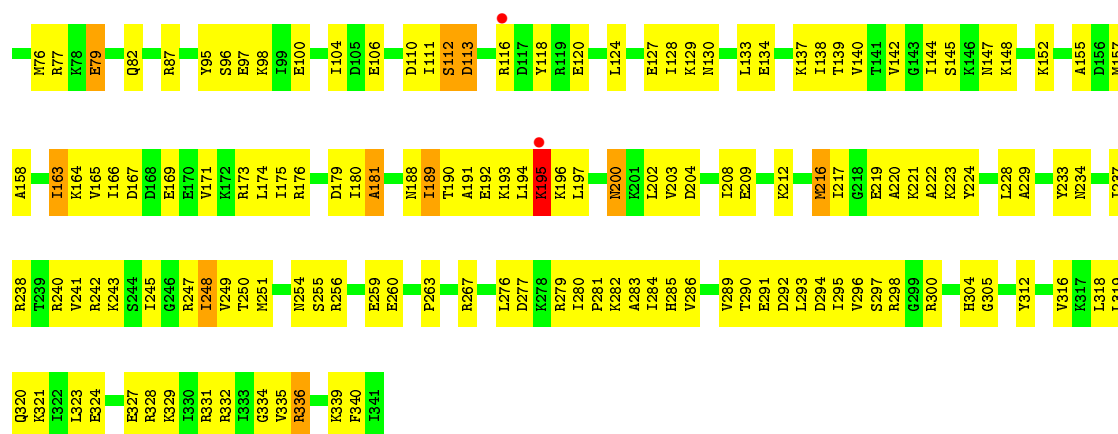
Chain F: 



- Molecule 3: DNA polymerase IV

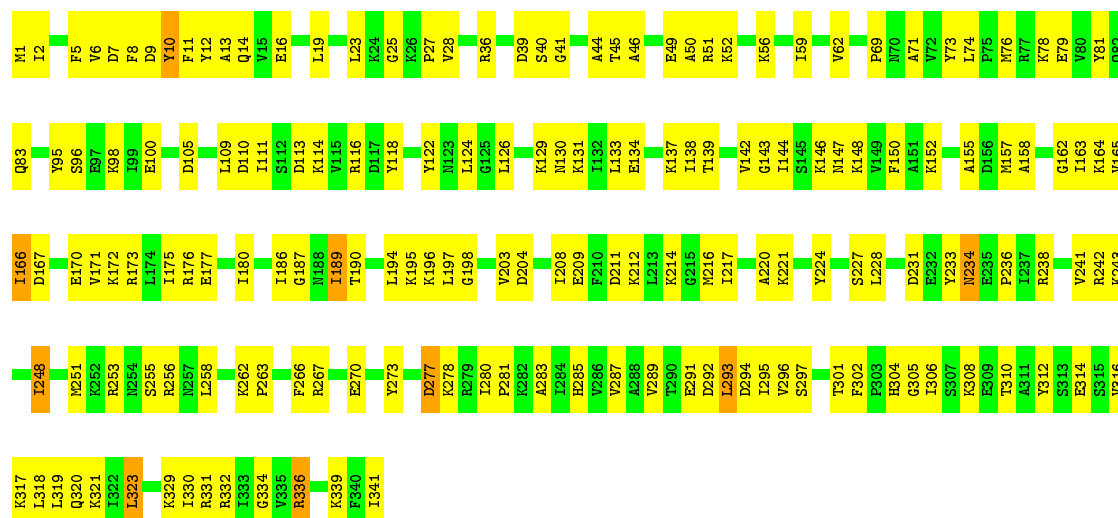
Chain A: 





• Molecule 3: DNA polymerase IV

Chain B: 50% 48%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.87Å 101.46Å 105.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.90) 93.7 (29.80-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.264 0.205 , 0.260	Depositor DCC
R_{free} test set	1121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7506	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5216e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, CA, MG, DGT

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	0.92	3/287 (1.0%)	1.13	5/444 (1.1%)
1	E	0.48	0/287	0.91	0/444
2	D	1.22	6/370 (1.6%)	1.63	10/567 (1.8%)
2	F	0.73	0/370	1.20	5/567 (0.9%)
3	A	0.45	1/2783 (0.0%)	0.66	2/3736 (0.1%)
3	B	0.40	0/2783	0.62	0/3736
All	All	0.55	10/6880 (0.1%)	0.81	22/9494 (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	1
2	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1904	DT	C3'-O3'	-8.52	1.32	1.44
2	D	1904	DT	O3'-P	-6.42	1.53	1.61
1	C	1809	DG	C2'-C1'	-6.26	1.46	1.52
2	D	1905	DT	C5-C6	-6.10	1.30	1.34
1	C	1812	DT	C4'-O4'	5.61	1.50	1.45
2	D	1903	DT	N3-C4	-5.49	1.34	1.38
2	D	1905	DT	O3'-P	-5.37	1.54	1.61
2	D	1903	DT	N1-C2	5.25	1.42	1.38
3	A	181	ALA	CA-CB	-5.23	1.41	1.52
1	C	1812	DT	C4'-C3'	5.04	1.58	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1903	DT	C2-N3-C4	-11.91	120.06	127.20
2	D	1903	DT	N3-C4-C5	11.43	122.06	115.20
1	C	1812	DT	O4'-C4'-C3'	8.21	110.93	106.00
3	A	195	LYS	C-N-CA	7.25	139.83	121.70
2	D	1903	DT	N1-C2-N3	6.92	118.75	114.60
2	D	1911	DC	C5'-C4'-O4'	-6.25	97.43	109.30
2	F	1903	DT	O4'-C1'-N1	6.21	112.34	108.00
2	F	1905	DT	C2-N1-C1'	6.09	127.95	118.20
2	F	1905	DT	C6-N1-C1'	-6.05	111.33	120.40
1	C	1812	DT	C4'-C3'-C2'	-6.03	97.67	103.10
2	D	1905	DT	P-O3'-C3'	6.03	126.94	119.70
2	F	1903	DT	C3'-C2'-C1'	-5.90	95.42	102.50
2	D	1906	DG	N9-C1'-C2'	5.78	123.58	112.60
1	C	1809	DG	C5'-C4'-C3'	-5.56	104.10	114.10
2	D	1903	DT	N3-C4-O4	-5.52	116.59	119.90
3	A	112	SER	N-CA-C	-5.45	96.28	111.00
1	C	1809	DG	O4'-C4'-C3'	-5.42	102.33	104.50
1	C	1812	DT	C1'-O4'-C4'	-5.38	104.72	110.10
2	D	1905	DT	O4'-C1'-C2'	-5.34	101.63	105.90
2	D	1905	DT	C2'-C3'-O3'	-5.09	95.79	112.60
2	D	1903	DT	C5-C4-O4	-5.07	121.35	124.90
2	F	1905	DT	C5'-C4'-O4'	5.05	118.89	109.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1910	DC	Sidechain
2	F	1903	DT	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	272	0	147	15	0
1	E	272	0	147	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	334	0	196	59	0
2	F	334	0	196	80	0
3	A	2744	0	2889	258	0
3	B	2744	0	2889	234	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	31	0	12	11	0
6	B	31	0	10	4	0
7	A	257	0	0	126	0
7	B	280	0	0	124	0
7	C	57	0	0	8	0
7	D	49	0	0	22	0
7	E	38	0	0	16	0
7	F	56	0	0	25	0
All	All	7506	0	6486	652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (652) 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)
2:D:1903:DT:H71	7:D:589:HOH:O	1.22	1.26
2:F:1902:DT:H3'	2:F:1903:DT:O4'	1.35	1.21
2:D:1903:DT:C7	7:D:589:HOH:O	1.77	1.17
2:F:1903:DT:C2'	2:F:1904:DT:H5'	1.76	1.16
2:F:1903:DT:H2''	2:F:1904:DT:H5'	1.26	1.13
2:D:1903:DT:H2'	2:D:1904:DT:C6	1.86	1.10
2:D:1903:DT:C7	7:D:884:HOH:O	2.01	1.08
2:D:1911:DC:H3'	7:D:964:HOH:O	1.53	1.05
2:D:1903:DT:H2''	2:D:1904:DT:H5'	1.35	1.04
3:A:194:LEU:O	3:A:196:LYS:N	1.90	1.03
3:A:63:GLU:HB2	7:A:879:HOH:O	1.58	1.03
2:F:1903:DT:C1'	2:F:1904:DT:H5'	1.89	1.03
2:D:1903:DT:H71	7:D:884:HOH:O	1.55	1.02
3:A:181:ALA:HB2	3:A:195:LYS:HE3	1.42	1.00
2:D:1903:DT:H2''	2:D:1904:DT:C5'	1.92	1.00
2:F:1903:DT:H2''	2:F:1904:DT:C5'	1.91	0.99
3:A:98:LYS:HB2	7:A:539:HOH:O	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:155:ALA:HB2	7:B:1149:HOH:O	1.62	0.97
3:A:245:ILE:HD12	3:A:276:LEU:HD23	1.46	0.97
3:B:256:ARG:HB2	3:B:323:LEU:HD11	1.46	0.96
3:A:202:LEU:HB3	7:A:1193:HOH:O	1.65	0.95
2:D:1905:DT:H5''	3:A:41:GLY:HA2	1.45	0.95
3:A:14:GLN:HE22	3:A:139:THR:H	1.05	0.94
2:F:1913:DT:H1'	2:F:1914:DC:H5'	1.50	0.94
2:D:1903:DT:C2'	2:D:1904:DT:H5'	1.97	0.93
1:E:1808:DG:H2''	7:E:1152:HOH:O	1.66	0.93
3:A:332:ARG:HG2	7:A:542:HOH:O	1.69	0.93
3:A:194:LEU:C	3:A:196:LYS:H	1.72	0.93
3:B:14:GLN:HE22	3:B:139:THR:H	1.01	0.92
3:B:332:ARG:HA	7:B:506:HOH:O	1.70	0.91
2:D:1903:DT:H2'	2:D:1904:DT:H6	1.34	0.90
3:B:14:GLN:HE22	3:B:139:THR:N	1.69	0.90
2:F:1902:DT:C3'	2:F:1903:DT:O4'	2.19	0.89
2:D:1903:DT:H2''	2:D:1904:DT:C4'	2.03	0.89
2:F:1905:DT:H2''	2:F:1906:DG:O4'	1.72	0.88
3:B:56:LYS:HE2	7:B:1100:HOH:O	1.73	0.88
2:D:1906:DG:H1'	7:D:743:HOH:O	1.70	0.88
3:B:186:ILE:HG12	7:B:1180:HOH:O	1.73	0.87
3:A:14:GLN:HE22	3:A:139:THR:N	1.72	0.87
3:A:248:ILE:HD11	3:A:332:ARG:HB3	1.55	0.87
3:A:221:LYS:HD3	7:A:551:HOH:O	1.75	0.87
3:B:289:VAL:HB	3:B:332:ARG:HB2	1.58	0.86
3:A:142:VAL:HG23	7:A:1140:HOH:O	1.76	0.85
7:F:1166:HOH:O	3:B:41:GLY:HA2	1.75	0.85
2:F:1903:DT:H2''	2:F:1904:DT:C3'	2.07	0.85
3:B:98:LYS:HB2	7:B:513:HOH:O	1.76	0.84
3:B:14:GLN:NE2	3:B:139:THR:H	1.75	0.84
3:A:196:LYS:HD3	7:A:519:HOH:O	1.77	0.84
2:F:1905:DT:H2'	2:F:1906:DG:C8	2.12	0.83
3:A:250:THR:HG23	7:A:542:HOH:O	1.80	0.82
3:B:248:ILE:HD11	3:B:332:ARG:HB3	1.62	0.82
3:A:296:VAL:HG23	7:A:1164:HOH:O	1.78	0.82
3:B:27:PRO:HB2	7:B:848:HOH:O	1.80	0.82
2:F:1906:DG:H2'	3:B:332:ARG:HH22	1.43	0.82
3:B:19:LEU:HB2	7:B:787:HOH:O	1.79	0.82
2:F:1912:DT:H72	7:F:1065:HOH:O	1.80	0.82
3:B:62:VAL:HG22	7:B:1092:HOH:O	1.81	0.81
1:E:1812:DT:H2''	1:E:1813:DOC:C5'	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1903:DT:H73	2:F:1904:DT:C7	2.10	0.81
3:A:155:ALA:HA	7:A:516:HOH:O	1.80	0.81
3:A:331:ARG:HD2	7:A:566:HOH:O	1.80	0.81
3:B:148:LYS:HB2	7:B:1215:HOH:O	1.80	0.80
1:E:1803:DG:H5''	7:E:1224:HOH:O	1.80	0.80
2:D:1903:DT:H5'	2:D:1904:DT:H72	1.61	0.80
7:E:1058:HOH:O	3:B:295:ILE:HD12	1.80	0.80
3:A:251:MET:HB3	7:A:1171:HOH:O	1.80	0.80
3:A:14:GLN:NE2	3:A:139:THR:H	1.79	0.79
3:A:247:ARG:HG3	7:A:1106:HOH:O	1.82	0.79
3:A:192:GLU:O	3:A:196:LYS:HB2	1.81	0.79
3:B:1:MET:HB3	7:B:1060:HOH:O	1.83	0.79
3:B:285:HIS:HB3	7:B:1134:HOH:O	1.83	0.79
3:A:51:ARG:NH2	6:A:401:DGT:O1G	2.16	0.78
1:E:1811:DT:H73	7:E:1058:HOH:O	1.83	0.78
3:B:329:LYS:HA	7:B:870:HOH:O	1.84	0.78
2:F:1903:DT:C7	2:F:1904:DT:H72	2.12	0.78
3:A:21:PRO:HG2	7:A:511:HOH:O	1.84	0.78
2:D:1909:DT:H2''	2:D:1910:DC:C6	2.19	0.77
2:F:1910:DC:H2''	2:F:1911:DC:O5'	1.85	0.77
3:A:134:GLU:HB3	7:A:766:HOH:O	1.84	0.77
3:A:112:SER:O	3:A:113:ASP:HB2	1.82	0.77
3:A:324:GLU:HB3	7:A:577:HOH:O	1.84	0.77
3:A:36:ARG:HD3	7:A:518:HOH:O	1.84	0.77
3:B:291:GLU:HB2	7:B:865:HOH:O	1.84	0.77
2:F:1903:DT:H1'	2:F:1904:DT:H5'	1.66	0.77
3:A:22:SER:HB3	7:A:899:HOH:O	1.85	0.77
3:A:179:ASP:OD1	3:A:195:LYS:HE2	1.85	0.76
3:B:256:ARG:HA	7:B:1184:HOH:O	1.85	0.76
3:A:97:GLU:OE1	3:A:97:GLU:N	2.17	0.76
3:A:242:ARG:HH11	3:A:242:ARG:HG3	1.51	0.76
3:B:96:SER:HB2	7:B:667:HOH:O	1.85	0.76
3:A:181:ALA:HB3	3:A:195:LYS:HZ1	1.50	0.76
3:A:28:VAL:HG22	7:A:1150:HOH:O	1.85	0.76
7:D:1086:HOH:O	3:A:62:VAL:HB	1.86	0.76
3:B:142:VAL:HG22	7:B:1073:HOH:O	1.85	0.75
1:E:1812:DT:H2''	1:E:1813:DOC:H5''	1.67	0.75
3:A:139:THR:HB	7:A:673:HOH:O	1.85	0.75
3:A:169:GLU:HB2	7:A:1018:HOH:O	1.87	0.75
2:D:1905:DT:OP2	3:A:331:ARG:NH2	2.18	0.75
3:B:180:ILE:HD13	3:B:194:LEU:HD13	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:341:ILE:HD11	7:B:1174:HOH:O	1.87	0.75
3:B:12:TYR:HB2	3:B:45:THR:HG21	1.68	0.74
3:B:157:MET:HE1	3:B:166:ILE:HD11	1.69	0.74
2:F:1907:DA:H2''	7:F:1145:HOH:O	1.86	0.74
2:D:1911:DC:O3'	3:A:220:ALA:HB3	1.88	0.74
3:B:45:THR:HG21	7:B:966:HOH:O	1.86	0.73
3:A:321:LYS:HE3	7:A:1222:HOH:O	1.87	0.73
3:B:256:ARG:HB3	7:B:870:HOH:O	1.87	0.73
3:A:248:ILE:HD13	3:A:249:VAL:N	2.03	0.73
3:A:12:TYR:HB2	3:A:45:THR:HG21	1.71	0.73
1:C:1804:DG:H2'	7:C:792:HOH:O	1.89	0.73
2:F:1903:DT:H73	2:F:1904:DT:H72	1.70	0.72
2:F:1911:DC:H2'	7:F:1065:HOH:O	1.88	0.72
2:F:1902:DT:H2'	2:F:1903:DT:C4'	2.19	0.72
3:B:146:LYS:HE2	7:B:1148:HOH:O	1.89	0.72
3:A:249:VAL:HG13	7:A:1106:HOH:O	1.88	0.72
3:B:69:PRO:HA	7:B:1022:HOH:O	1.88	0.72
2:D:1906:DG:H2'	3:A:332:ARG:HH22	1.55	0.72
7:E:612:HOH:O	2:F:1911:DC:H1'	1.89	0.71
3:A:248:ILE:HA	3:A:334:GLY:HA3	1.72	0.71
3:B:157:MET:CE	3:B:166:ILE:HD11	2.21	0.71
3:B:283:ALA:HB2	3:B:339:LYS:HD2	1.72	0.71
3:B:227:SER:HB2	7:B:872:HOH:O	1.89	0.71
2:D:1913:DT:H5'	7:D:840:HOH:O	1.90	0.71
3:B:79:GLU:HB3	7:B:1068:HOH:O	1.89	0.71
3:A:300:ARG:HB2	7:A:1124:HOH:O	1.89	0.71
2:F:1904:DT:H1'	2:F:1905:DT:OP2	1.90	0.71
3:A:111:ILE:HA	7:A:592:HOH:O	1.90	0.71
3:B:118:TYR:HE1	7:B:630:HOH:O	1.74	0.71
3:B:336:ARG:HD2	7:B:811:HOH:O	1.90	0.70
2:F:1902:DT:H2'	2:F:1903:DT:H4'	1.71	0.70
2:D:1912:DT:H1'	7:D:840:HOH:O	1.92	0.70
2:F:1903:DT:H2''	2:F:1904:DT:C4'	2.20	0.70
2:F:1916:DC:H1'	2:F:1917:DC:H5'	1.73	0.70
3:B:236:PRO:HG2	3:B:238:ARG:HH11	1.57	0.70
2:F:1907:DA:H1'	7:F:700:HOH:O	1.91	0.70
3:B:131:LYS:HG2	7:B:1063:HOH:O	1.92	0.69
3:A:196:LYS:CD	7:A:519:HOH:O	2.37	0.69
3:B:6:VAL:HA	7:B:1073:HOH:O	1.92	0.69
3:A:290:THR:HG23	7:A:1164:HOH:O	1.92	0.69
3:A:116:ARG:HB2	7:A:713:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1915:DC:H5''	7:F:531:HOH:O	1.91	0.69
3:B:173:ARG:HB2	7:B:997:HOH:O	1.93	0.69
3:A:130:ASN:HB2	7:A:756:HOH:O	1.93	0.68
7:F:631:HOH:O	3:B:36:ARG:HD2	1.93	0.68
3:B:211:ASP:HB3	7:B:624:HOH:O	1.92	0.68
3:A:175:ILE:HG23	7:A:1193:HOH:O	1.93	0.68
3:A:3:VAL:HG22	7:A:1159:HOH:O	1.92	0.68
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.75	0.68
2:F:1904:DT:OP1	3:B:40:SER:HA	1.93	0.68
3:A:45:THR:HG21	7:A:1160:HOH:O	1.94	0.67
3:B:248:ILE:C	3:B:248:ILE:HD13	2.14	0.67
3:B:114:LYS:HG2	7:B:1157:HOH:O	1.94	0.67
1:E:1811:DT:H71	7:E:866:HOH:O	1.93	0.67
3:A:255:SER:HB2	7:A:778:HOH:O	1.95	0.67
3:A:285:HIS:HD2	7:A:720:HOH:O	1.78	0.67
3:B:110:ASP:O	7:B:513:HOH:O	2.12	0.67
3:A:157:MET:CE	3:A:166:ILE:HD11	2.24	0.67
3:A:248:ILE:HD11	3:A:332:ARG:CB	2.25	0.67
3:B:242:ARG:HG3	3:B:242:ARG:HH11	1.59	0.67
3:B:216:MET:HA	3:B:216:MET:HE2	1.75	0.67
3:B:109:LEU:HD23	7:B:667:HOH:O	1.95	0.66
3:B:312:TYR:O	3:B:316:VAL:HG23	1.95	0.66
3:B:116:ARG:HB3	3:B:116:ARG:NH1	2.10	0.66
3:A:112:SER:O	3:A:113:ASP:CB	2.42	0.66
3:A:181:ALA:HB2	3:A:195:LYS:CE	2.23	0.66
3:A:248:ILE:CD1	3:A:332:ARG:HB3	2.26	0.66
3:B:129:LYS:HE2	7:B:670:HOH:O	1.94	0.66
3:A:289:VAL:HG13	7:A:1125:HOH:O	1.94	0.66
1:C:1806:DA:H5''	7:C:557:HOH:O	1.95	0.66
3:B:16:GLU:HA	7:B:787:HOH:O	1.95	0.66
3:B:148:LYS:HE3	7:B:1215:HOH:O	1.96	0.66
7:E:917:HOH:O	3:B:189:ILE:HD12	1.96	0.66
1:E:1806:DA:H5''	7:E:1059:HOH:O	1.96	0.65
3:B:195:LYS:CG	7:B:1050:HOH:O	2.44	0.65
3:B:2:ILE:HA	7:B:630:HOH:O	1.96	0.65
2:F:1903:DT:H73	2:F:1904:DT:H73	1.77	0.65
3:B:143:GLY:HA3	7:B:1149:HOH:O	1.96	0.65
3:A:98:LYS:HA	7:A:527:HOH:O	1.97	0.65
3:B:241:VAL:HA	7:B:765:HOH:O	1.96	0.65
3:A:10:TYR:HA	6:A:401:DGT:O2G	1.97	0.65
2:D:1907:DA:OP2	3:A:248:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:ASN:N	3:A:200:ASN:HD22	1.95	0.65
3:B:233:TYR:HB3	7:B:530:HOH:O	1.96	0.65
1:C:1807:DA:H2''	1:C:1808:DG:OP2	1.97	0.65
3:A:335:VAL:HG22	7:A:1190:HOH:O	1.97	0.65
3:B:162:GLY:HA3	7:B:699:HOH:O	1.96	0.65
3:B:110:ASP:HB3	7:B:513:HOH:O	1.96	0.64
3:B:292:ASP:O	3:B:293:LEU:HB2	1.95	0.64
3:B:79:GLU:H	3:B:79:GLU:CD	1.96	0.64
3:A:194:LEU:C	3:A:196:LYS:N	2.43	0.64
2:D:1905:DT:H6	7:D:747:HOH:O	1.81	0.64
1:E:1813:DOC:C2	2:F:1906:DG:H22	2.10	0.64
1:E:1809:DG:H1'	1:E:1810:DA:H5'	1.80	0.64
2:D:1906:DG:H2'	3:A:332:ARG:NH2	2.12	0.64
2:F:1905:DT:C2'	2:F:1906:DG:C8	2.80	0.64
3:A:229:ALA:HA	7:A:1193:HOH:O	1.97	0.64
3:A:36:ARG:HG3	7:A:1182:HOH:O	1.98	0.64
1:E:1804:DG:H2'	7:E:653:HOH:O	1.98	0.64
3:A:69:PRO:HA	7:A:524:HOH:O	1.97	0.63
3:A:202:LEU:HB2	7:A:1155:HOH:O	1.98	0.63
2:F:1903:DT:H2''	2:F:1904:DT:H3'	1.78	0.63
3:B:195:LYS:HG3	7:B:1050:HOH:O	1.98	0.63
3:B:233:TYR:HA	7:B:872:HOH:O	1.98	0.63
3:B:321:LYS:HD3	7:B:757:HOH:O	1.98	0.63
3:A:49:GLU:HA	3:A:52:LYS:HE2	1.79	0.63
3:A:248:ILE:HG21	7:A:1179:HOH:O	1.98	0.62
3:A:95:TYR:CD1	3:A:124:LEU:HD11	2.34	0.62
2:F:1903:DT:H71	2:F:1904:DT:H72	1.80	0.62
3:A:263:PRO:O	3:A:267:ARG:HG3	1.99	0.62
1:E:1810:DA:H2''	7:E:866:HOH:O	1.99	0.62
3:A:221:LYS:HB2	7:A:504:HOH:O	1.99	0.62
3:A:318:LEU:HD21	7:A:1124:HOH:O	1.99	0.62
3:B:78:LYS:HG2	7:B:1176:HOH:O	1.99	0.62
3:A:148:LYS:HG3	7:A:1221:HOH:O	1.99	0.62
3:A:240:ARG:HB3	7:A:629:HOH:O	1.99	0.62
2:F:1903:DT:H2'	7:B:1217:HOH:O	1.98	0.62
3:A:79:GLU:H	3:A:79:GLU:CD	2.02	0.62
3:B:195:LYS:HB2	7:B:981:HOH:O	2.00	0.62
3:B:39:ASP:HB2	7:B:1092:HOH:O	1.98	0.62
3:A:171:VAL:O	3:A:175:ILE:HG13	1.99	0.61
3:B:251:MET:N	7:B:506:HOH:O	2.32	0.61
2:D:1904:DT:H3'	2:D:1904:DT:P	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:195:LYS:CD	7:B:1050:HOH:O	2.48	0.61
1:E:1802:DG:H2'	7:E:869:HOH:O	2.00	0.61
3:A:256:ARG:HG3	7:A:856:HOH:O	1.99	0.61
3:A:181:ALA:CB	3:A:195:LYS:HE3	2.23	0.61
3:A:111:ILE:HG22	7:A:592:HOH:O	2.00	0.61
3:B:171:VAL:O	3:B:175:ILE:HG13	2.01	0.61
2:F:1904:DT:H71	7:F:1101:HOH:O	2.01	0.61
1:E:1813:DOC:C4	2:F:1906:DG:H1	2.14	0.61
3:A:96:SER:HB2	7:A:592:HOH:O	2.00	0.61
3:B:111:ILE:HA	7:B:1157:HOH:O	2.01	0.61
3:B:336:ARG:NH1	7:B:875:HOH:O	2.33	0.61
3:A:320:GLN:HA	7:A:1203:HOH:O	1.99	0.60
3:B:12:TYR:HB2	3:B:45:THR:CG2	2.32	0.60
3:B:95:TYR:HD1	3:B:124:LEU:HD11	1.66	0.60
2:F:1906:DG:H2'	3:B:332:ARG:NH2	2.14	0.60
3:A:110:ASP:HB3	7:A:539:HOH:O	2.00	0.60
3:A:157:MET:HE1	3:A:166:ILE:HD11	1.83	0.60
3:A:241:VAL:HA	7:A:655:HOH:O	2.01	0.60
3:B:133:LEU:HD12	3:B:137:LYS:HA	1.82	0.60
3:B:253:ARG:HD3	7:B:534:HOH:O	2.01	0.60
2:D:1906:DG:N2	7:D:864:HOH:O	2.31	0.60
3:A:197:LEU:HD22	7:A:1194:HOH:O	2.01	0.60
3:A:72:VAL:HB	7:A:1150:HOH:O	2.00	0.60
3:A:127:GLU:HB2	7:A:1214:HOH:O	2.01	0.59
2:D:1908:DA:H2'	3:A:336:ARG:NH2	2.17	0.59
3:A:216:MET:HE2	3:A:216:MET:HA	1.84	0.59
3:B:14:GLN:NE2	3:B:138:ILE:HA	2.16	0.59
3:B:76:MET:HG2	3:B:81:TYR:HE2	1.68	0.59
3:A:147:ASN:HB2	7:A:1017:HOH:O	2.01	0.59
3:A:144:ILE:HB	3:A:165:VAL:HG22	1.85	0.59
3:B:95:TYR:CD1	3:B:124:LEU:HD11	2.37	0.59
3:A:95:TYR:HD1	3:A:124:LEU:HD11	1.68	0.58
3:B:256:ARG:HD2	7:B:870:HOH:O	2.02	0.58
2:D:1904:DT:OP2	2:D:1904:DT:H3'	2.03	0.58
1:E:1809:DG:H8	7:E:1152:HOH:O	1.85	0.58
3:B:243:LYS:HD3	7:B:553:HOH:O	2.02	0.58
3:B:293:LEU:HB3	7:B:1189:HOH:O	2.01	0.58
3:B:36:ARG:NH1	3:B:331:ARG:NH1	2.52	0.58
3:B:36:ARG:HA	7:B:614:HOH:O	2.03	0.58
1:C:1813:DOC:H1'	7:C:1049:HOH:O	2.01	0.58
2:F:1911:DC:H5''	7:F:1065:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:GLU:OE2	7:A:713:HOH:O	2.16	0.58
3:B:113:ASP:O	3:B:114:LYS:HD3	2.03	0.58
3:B:197:LEU:HD22	3:B:212:LYS:HE2	1.85	0.58
3:B:341:ILE:HG22	3:B:341:ILE:OXT	2.04	0.58
1:E:1812:DT:H2''	1:E:1813:DOC:H5'	1.86	0.58
2:F:1907:DA:H1'	7:F:1145:HOH:O	2.02	0.58
3:A:219:GLU:O	3:A:223:LYS:HG3	2.02	0.58
3:A:329:LYS:HD2	7:A:561:HOH:O	2.02	0.58
3:B:256:ARG:NH2	3:B:323:LEU:HD12	2.19	0.58
2:F:1902:DT:H5''	2:F:1903:DT:N1	2.18	0.58
3:A:237:ILE:N	3:A:237:ILE:HD12	2.19	0.58
3:A:238:ARG:HD3	7:A:941:HOH:O	2.03	0.58
3:A:292:ASP:OD1	3:A:328:ARG:HD2	2.03	0.58
3:B:253:ARG:CD	7:B:534:HOH:O	2.51	0.58
3:B:6:VAL:HG13	7:B:1073:HOH:O	2.03	0.58
2:D:1905:DT:H4'	2:D:1906:DG:OP1	2.02	0.57
3:A:282:LYS:HG3	7:A:1141:HOH:O	2.04	0.57
3:B:289:VAL:HB	3:B:332:ARG:CB	2.33	0.57
2:F:1904:DT:OP1	3:B:40:SER:HB2	2.04	0.57
3:B:273:TYR:HE1	7:B:730:HOH:O	1.87	0.57
3:A:129:LYS:HG2	7:A:1144:HOH:O	2.04	0.57
1:E:1809:DG:H1'	1:E:1810:DA:C5'	2.35	0.57
3:A:180:ILE:HD13	3:A:194:LEU:HD13	1.86	0.57
2:F:1907:DA:C2'	7:F:1145:HOH:O	2.47	0.57
2:D:1911:DC:H2''	2:D:1912:DT:O5'	2.05	0.57
3:A:321:LYS:HB2	7:A:1222:HOH:O	2.05	0.57
2:F:1902:DT:H3'	2:F:1903:DT:C4'	2.35	0.57
3:A:260:GLU:HG2	7:A:550:HOH:O	2.05	0.56
3:B:289:VAL:CB	3:B:332:ARG:HB2	2.34	0.56
3:A:36:ARG:NH2	3:A:254:ASN:OD1	2.34	0.56
3:B:9:ASP:O	3:B:11:PHE:N	2.38	0.56
3:A:14:GLN:NE2	3:A:138:ILE:HA	2.20	0.56
3:A:163:ILE:HG13	7:A:625:HOH:O	2.06	0.56
3:A:284:ILE:HG13	7:A:1190:HOH:O	2.06	0.56
3:A:197:LEU:O	7:A:567:HOH:O	2.17	0.56
1:C:1813:DOC:H2''	6:A:401:DGT:O4'	2.05	0.56
1:C:1802:DG:H2'	7:C:703:HOH:O	2.05	0.55
2:D:1903:DT:H73	7:D:884:HOH:O	1.82	0.55
3:A:148:LYS:HE2	7:A:1221:HOH:O	2.05	0.55
3:A:60:PRO:HD2	7:A:879:HOH:O	2.06	0.55
3:B:208:ILE:HG12	3:B:209:GLU:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1810:DA:H5''	7:C:583:HOH:O	2.05	0.55
3:B:267:ARG:HD2	7:B:759:HOH:O	2.05	0.55
2:D:1908:DA:P	3:A:336:ARG:HH22	2.30	0.55
3:B:242:ARG:HD2	7:B:886:HOH:O	2.06	0.55
2:D:1903:DT:H5'	2:D:1904:DT:C7	2.34	0.55
2:D:1903:DT:H2''	2:D:1904:DT:O4'	2.06	0.55
3:A:157:MET:HE1	3:A:164:LYS:HE3	1.88	0.55
3:B:280:ILE:HB	7:B:1170:HOH:O	2.07	0.55
1:C:1808:DG:H1	2:D:1911:DC:H42	1.55	0.55
3:B:176:ARG:NH1	7:B:940:HOH:O	2.40	0.55
3:A:25:GLY:O	3:A:49:GLU:HG2	2.08	0.54
3:A:62:VAL:HA	7:A:1143:HOH:O	2.07	0.54
3:B:144:ILE:HB	3:B:165:VAL:HG22	1.89	0.54
1:E:1811:DT:H5'	7:E:677:HOH:O	2.06	0.54
2:F:1902:DT:C2'	2:F:1903:DT:C4'	2.84	0.54
2:F:1913:DT:C1'	2:F:1914:DC:H5'	2.30	0.54
3:A:130:ASN:HA	7:A:1088:HOH:O	2.07	0.54
3:A:130:ASN:HB3	7:A:854:HOH:O	2.08	0.54
3:A:140:VAL:HG22	7:A:1144:HOH:O	2.06	0.54
2:F:1913:DT:H2''	2:F:1914:DC:O5'	2.07	0.54
3:B:143:GLY:N	7:B:1149:HOH:O	2.39	0.54
2:D:1905:DT:H5'	7:D:747:HOH:O	2.07	0.54
3:A:12:TYR:HB2	3:A:45:THR:CG2	2.36	0.54
3:A:295:ILE:CG1	7:A:1125:HOH:O	2.54	0.54
3:B:5:PHE:HD2	7:B:1149:HOH:O	1.91	0.54
3:A:116:ARG:HG2	7:A:1183:HOH:O	2.07	0.54
3:B:143:GLY:CA	7:B:1149:HOH:O	2.54	0.54
6:A:401:DGT:H5'	6:A:401:DGT:O3B	2.08	0.54
2:F:1902:DT:H5''	2:F:1903:DT:C2	2.43	0.54
3:A:191:ALA:O	3:A:195:LYS:N	2.40	0.53
3:B:251:MET:HG3	7:B:506:HOH:O	2.08	0.53
1:E:1812:DT:C2'	1:E:1813:DOC:H5'	2.38	0.53
2:F:1902:DT:C2'	2:F:1903:DT:H5'	2.38	0.53
3:A:157:MET:HE2	3:A:166:ILE:HD11	1.90	0.53
3:A:242:ARG:NH1	3:A:242:ARG:HG3	2.22	0.53
3:B:118:TYR:HB3	3:B:165:VAL:HG11	1.90	0.53
3:A:327:GLU:N	7:A:1158:HOH:O	2.41	0.53
3:A:332:ARG:NH2	7:A:1179:HOH:O	2.38	0.53
3:A:295:ILE:HG13	7:A:1125:HOH:O	2.07	0.53
3:B:305:GLY:N	7:B:1174:HOH:O	2.42	0.53
2:D:1917:DC:H3'	7:D:744:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:36:ARG:NH1	3:B:331:ARG:HH12	2.07	0.53
3:A:113:ASP:HB3	7:A:674:HOH:O	2.08	0.53
3:A:336:ARG:HD2	7:A:676:HOH:O	2.08	0.53
3:B:317:LYS:HE3	7:B:1142:HOH:O	2.08	0.53
2:F:1904:DT:OP1	3:B:40:SER:CA	2.57	0.53
1:C:1813:DOC:H5'	3:A:106:GLU:OE1	2.09	0.52
1:E:1803:DG:C5'	7:E:1224:HOH:O	2.47	0.52
3:B:131:LYS:HE3	7:B:1063:HOH:O	2.08	0.52
3:B:308:LYS:O	3:B:312:TYR:HD2	1.92	0.52
3:A:320:GLN:O	3:A:324:GLU:HG3	2.10	0.52
2:F:1907:DA:H2'	7:B:875:HOH:O	2.10	0.52
3:A:142:VAL:N	7:A:1140:HOH:O	2.41	0.52
3:B:122:TYR:CE2	3:B:126:LEU:HD11	2.43	0.52
3:B:332:ARG:NH1	7:B:1185:HOH:O	2.42	0.52
2:F:1908:DA:P	3:B:336:ARG:HH22	2.32	0.52
3:B:28:VAL:HG22	7:B:565:HOH:O	2.09	0.52
3:A:10:TYR:HA	6:A:401:DGT:PG	2.49	0.52
2:D:1908:DA:H2'	3:A:336:ARG:HH21	1.74	0.52
2:F:1908:DA:O4'	7:F:1145:HOH:O	2.19	0.52
3:A:100:GLU:HB2	3:A:237:ILE:HG23	1.91	0.52
3:A:76:MET:HE1	6:A:401:DGT:N2	2.25	0.52
3:A:133:LEU:HD12	3:A:137:LYS:HA	1.92	0.52
3:A:190:THR:HG23	7:A:892:HOH:O	2.10	0.52
3:A:116:ARG:CG	7:A:1183:HOH:O	2.57	0.52
3:A:98:LYS:HE3	7:A:1226:HOH:O	2.09	0.52
3:B:236:PRO:HG2	3:B:238:ARG:NH1	2.24	0.52
1:E:1809:DG:N3	1:E:1810:DA:O4'	2.42	0.52
3:B:195:LYS:HD2	7:B:1050:HOH:O	2.07	0.51
3:B:293:LEU:HD22	7:B:1189:HOH:O	2.09	0.51
3:A:283:ALA:HB2	3:A:339:LYS:HD2	1.91	0.51
3:A:118:TYR:HB3	3:A:165:VAL:HG11	1.91	0.51
3:A:76:MET:HE1	6:A:401:DGT:HN2A	1.75	0.51
3:A:312:TYR:O	3:A:316:VAL:HG23	2.11	0.51
2:D:1903:DT:H72	7:D:589:HOH:O	1.72	0.51
3:A:243:LYS:NZ	7:A:1162:HOH:O	2.40	0.51
3:A:321:LYS:HD3	7:A:533:HOH:O	2.08	0.51
3:A:129:LYS:HD2	7:A:1140:HOH:O	2.09	0.51
2:F:1905:DT:H73	7:F:1199:HOH:O	2.09	0.51
6:A:401:DGT:H8	6:A:401:DGT:H5'A	1.93	0.51
1:C:1809:DG:H4'	7:C:1198:HOH:O	2.11	0.51
3:A:173:ARG:HD3	7:A:885:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:ILE:HD12	7:A:1194:HOH:O	2.10	0.51
3:B:253:ARG:NH1	7:B:534:HOH:O	2.44	0.51
3:B:49:GLU:HA	3:B:52:LYS:HE2	1.92	0.51
2:F:1904:DT:H73	7:F:896:HOH:O	2.11	0.51
3:B:296:VAL:HA	7:B:582:HOH:O	2.10	0.50
3:A:179:ASP:OD1	3:A:195:LYS:CE	2.57	0.50
3:B:304:HIS:HA	7:B:626:HOH:O	2.11	0.50
2:D:1903:DT:H2''	2:D:1904:DT:C3'	2.42	0.50
2:D:1904:DT:C4	3:A:293:LEU:CD1	2.95	0.50
3:A:65:LYS:HD2	7:A:1143:HOH:O	2.11	0.50
2:D:1903:DT:C2'	2:D:1904:DT:C6	2.78	0.50
2:F:1904:DT:OP1	3:B:40:SER:CB	2.59	0.50
3:A:152:LYS:NZ	7:A:1048:HOH:O	2.43	0.50
3:A:248:ILE:HD13	3:A:248:ILE:C	2.32	0.50
3:A:304:HIS:HD2	3:A:305:GLY:O	1.94	0.50
2:D:1909:DT:H2''	2:D:1910:DC:H6	1.74	0.50
2:F:1911:DC:H2''	2:F:1912:DT:O5'	2.10	0.50
3:A:76:MET:CE	6:A:401:DGT:N2	2.75	0.49
3:B:280:ILE:C	7:B:525:HOH:O	2.51	0.49
3:B:316:VAL:O	3:B:320:GLN:HG3	2.12	0.49
1:C:1811:DT:OP2	3:A:189:ILE:HB	2.12	0.49
3:A:327:GLU:HB3	7:A:1158:HOH:O	2.12	0.49
2:F:1904:DT:O3'	7:F:1166:HOH:O	2.19	0.49
3:A:40:SER:N	7:A:785:HOH:O	2.46	0.49
3:B:285:HIS:HD2	7:B:974:HOH:O	1.95	0.49
3:A:181:ALA:CB	3:A:195:LYS:HZ1	2.21	0.49
3:A:22:SER:CB	7:A:1098:HOH:O	2.60	0.49
3:B:130:ASN:HB3	7:B:1034:HOH:O	2.13	0.49
3:A:281:PRO:C	7:A:1141:HOH:O	2.51	0.49
3:B:231:ASP:HB3	7:B:850:HOH:O	2.11	0.49
3:A:104:ILE:HG22	7:A:724:HOH:O	2.12	0.49
3:B:148:LYS:HG3	7:B:799:HOH:O	2.12	0.49
3:B:248:ILE:HA	3:B:334:GLY:HA3	1.93	0.49
2:F:1902:DT:C2'	2:F:1903:DT:C5'	2.90	0.49
3:B:122:TYR:HE2	3:B:126:LEU:HD11	1.76	0.49
3:B:214:LYS:HD3	7:B:532:HOH:O	2.13	0.49
2:D:1903:DT:C1'	2:D:1904:DT:H5'	2.42	0.49
2:D:1916:DC:H3'	7:D:1020:HOH:O	2.13	0.49
3:B:7:ASP:CG	7:B:1051:HOH:O	2.50	0.48
2:F:1911:DC:C5'	7:F:1053:HOH:O	2.61	0.48
3:B:10:TYR:HD1	3:B:13:ALA:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1912:DT:H3'	7:F:913:HOH:O	2.12	0.48
3:A:44:ALA:CB	3:A:76:MET:HE2	2.42	0.48
3:B:164:LYS:CG	3:B:165:VAL:N	2.76	0.48
3:A:237:ILE:N	3:A:237:ILE:CD1	2.76	0.48
3:B:9:ASP:O	3:B:10:TYR:C	2.51	0.48
3:B:256:ARG:CZ	3:B:323:LEU:HD12	2.44	0.48
3:A:8:PHE:N	3:A:8:PHE:CD1	2.79	0.48
2:D:1914:DC:H2''	2:D:1915:DC:C6	2.49	0.48
2:F:1903:DT:H2''	2:F:1904:DT:C2'	2.44	0.48
3:A:200:ASN:ND2	3:A:200:ASN:N	2.61	0.48
3:A:233:TYR:HA	7:A:1081:HOH:O	2.14	0.48
3:A:319:LEU:HB3	7:A:520:HOH:O	2.12	0.48
3:A:56:LYS:NZ	7:A:833:HOH:O	2.46	0.48
3:A:188:ASN:N	3:A:188:ASN:HD22	2.11	0.48
7:D:855:HOH:O	3:A:240:ARG:HD3	2.12	0.48
6:A:401:DGT:O1B	6:A:401:DGT:O1G	2.30	0.48
3:B:134:GLU:HG2	7:B:936:HOH:O	2.13	0.48
3:B:170:GLU:HA	7:B:997:HOH:O	2.14	0.48
2:D:1904:DT:H5''	3:A:60:PRO:HG3	1.96	0.48
3:A:87:ARG:HD3	7:A:596:HOH:O	2.14	0.48
3:B:100:GLU:HG3	3:B:238:ARG:O	2.13	0.48
3:B:248:ILE:HD11	3:B:332:ARG:CB	2.39	0.48
3:B:267:ARG:HD2	7:B:512:HOH:O	2.14	0.47
3:A:208:ILE:HG12	3:A:209:GLU:N	2.28	0.47
3:A:217:ILE:HD11	3:A:222:ALA:HA	1.96	0.47
3:A:282:LYS:N	7:A:1141:HOH:O	2.46	0.47
3:B:157:MET:HE2	3:B:166:ILE:HD11	1.97	0.47
3:B:319:LEU:HD12	3:B:319:LEU:O	2.14	0.47
3:B:329:LYS:HG2	7:B:870:HOH:O	2.14	0.47
3:B:23:LEU:HD22	7:B:565:HOH:O	2.14	0.47
7:F:973:HOH:O	3:B:76:MET:HE1	2.13	0.47
2:F:1906:DG:H4'	7:F:1195:HOH:O	2.12	0.47
3:B:164:LYS:HG3	3:B:165:VAL:N	2.28	0.47
3:B:233:TYR:HE2	7:B:1215:HOH:O	1.97	0.47
3:B:281:PRO:N	7:B:525:HOH:O	2.48	0.47
7:F:1188:HOH:O	3:B:295:ILE:HD11	2.14	0.47
3:B:8:PHE:N	3:B:8:PHE:CD1	2.80	0.47
3:A:110:ASP:HA	7:A:1159:HOH:O	2.14	0.47
3:A:73:TYR:N	7:A:1062:HOH:O	2.42	0.47
3:B:79:GLU:O	3:B:83:GLN:HG3	2.15	0.47
1:C:1808:DG:H1	2:D:1911:DC:N4	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1902:DT:H2''	2:F:1903:DT:H5'	1.95	0.47
3:A:116:ARG:HD3	7:A:1183:HOH:O	2.13	0.47
3:B:111:ILE:HG22	7:B:667:HOH:O	2.14	0.47
1:E:1806:DA:H2''	1:E:1807:DA:C8	2.50	0.47
2:F:1905:DT:H2''	2:F:1906:DG:C1'	2.44	0.47
3:B:262:LYS:HB2	3:B:263:PRO:HD3	1.96	0.47
3:B:234:ASN:HD22	3:B:234:ASN:HA	1.52	0.47
1:C:1808:DG:H3'	7:C:1163:HOH:O	2.15	0.47
2:F:1916:DC:H2''	2:F:1917:DC:O5'	2.14	0.47
3:A:116:ARG:CZ	3:A:116:ARG:HB3	2.45	0.46
3:A:166:ILE:HD12	3:A:174:LEU:HD11	1.97	0.46
3:A:9:ASP:O	3:A:10:TYR:C	2.52	0.46
3:A:130:ASN:O	3:A:134:GLU:HG3	2.15	0.46
2:D:1906:DG:P	7:D:1206:HOH:O	2.72	0.46
2:F:1903:DT:H1'	2:F:1904:DT:C5'	2.41	0.46
3:A:242:ARG:HH11	3:A:242:ARG:CG	2.24	0.46
3:A:319:LEU:HD12	3:A:319:LEU:O	2.16	0.46
3:B:177:GLU:HG2	7:B:829:HOH:O	2.13	0.46
2:D:1911:DC:O3'	3:A:220:ALA:CB	2.62	0.46
3:A:3:VAL:O	3:A:144:ILE:HA	2.15	0.46
3:A:197:LEU:HB3	7:A:1194:HOH:O	2.15	0.46
3:B:146:LYS:HG3	7:B:1148:HOH:O	2.14	0.46
3:B:56:LYS:O	3:B:59:ILE:HG12	2.15	0.46
2:F:1911:DC:H3'	7:F:742:HOH:O	2.16	0.46
3:A:124:LEU:O	3:A:128:ILE:HG13	2.16	0.46
3:A:217:ILE:HD12	3:A:221:LYS:HB3	1.97	0.46
3:A:22:SER:HB2	7:A:1098:HOH:O	2.15	0.46
3:A:9:ASP:O	3:A:11:PHE:N	2.49	0.46
3:B:73:TYR:O	3:B:74:LEU:HD23	2.16	0.46
3:B:118:TYR:CE2	3:B:167:ASP:HA	2.51	0.46
7:F:1053:HOH:O	3:B:220:ALA:HB2	2.16	0.46
3:B:330:ILE:HG13	7:B:1184:HOH:O	2.15	0.46
2:F:1903:DT:C7	2:F:1904:DT:C7	2.80	0.45
3:B:2:ILE:HG23	7:B:630:HOH:O	2.14	0.45
3:B:147:ASN:HD21	3:B:150:PHE:HD2	1.64	0.45
2:D:1904:DT:H1'	7:D:747:HOH:O	2.15	0.45
2:D:1908:DA:H2''	2:D:1909:DT:OP2	2.16	0.45
3:A:56:LYS:O	3:A:59:ILE:HG12	2.15	0.45
3:B:1:MET:HE3	7:B:799:HOH:O	2.15	0.45
6:B:501:DGT:H8	6:B:501:DGT:O5'	2.16	0.45
1:E:1809:DG:C2	1:E:1810:DA:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1904:DT:C4	3:A:293:LEU:HD11	2.50	0.45
3:B:289:VAL:HG21	3:B:332:ARG:HD3	1.98	0.45
2:D:1914:DC:H2'	2:D:1915:DC:H6	1.82	0.45
3:A:254:ASN:HD22	3:A:291:GLU:HB3	1.82	0.45
3:B:23:LEU:CD2	7:B:565:HOH:O	2.65	0.45
3:A:164:LYS:HG3	3:A:165:VAL:N	2.32	0.45
3:A:224:TYR:CZ	3:A:228:LEU:HD11	2.52	0.45
2:F:1903:DT:C2'	2:F:1904:DT:H2'	2.47	0.45
3:A:176:ARG:NH1	7:A:732:HOH:O	2.49	0.45
3:B:114:LYS:HE2	7:B:951:HOH:O	2.17	0.45
7:F:529:HOH:O	3:B:293:LEU:CD2	2.65	0.45
1:C:1810:DA:N7	7:C:1054:HOH:O	2.36	0.45
3:B:208:ILE:CG1	3:B:209:GLU:N	2.79	0.44
3:B:220:ALA:HB3	7:B:754:HOH:O	2.16	0.44
3:B:302:PHE:C	3:B:304:HIS:H	2.20	0.44
3:B:98:LYS:HB2	3:B:110:ASP:HB3	1.98	0.44
3:B:304:HIS:HD2	3:B:305:GLY:O	1.99	0.44
3:B:331:ARG:NH2	7:B:1217:HOH:O	2.49	0.44
3:B:71:ALA:HB1	7:B:848:HOH:O	2.17	0.44
1:C:1801:DG:H2'	3:B:83:GLN:OE1	2.16	0.44
2:F:1909:DT:H3'	7:B:574:HOH:O	2.18	0.44
3:B:158:ALA:HB1	7:B:699:HOH:O	2.16	0.44
3:A:38:GLU:HG2	7:A:895:HOH:O	2.17	0.44
3:B:163:ILE:O	3:B:163:ILE:HG23	2.17	0.44
3:A:82:GLN:HB2	7:A:600:HOH:O	2.17	0.44
1:E:1807:DA:H2'	7:B:898:HOH:O	2.18	0.44
3:B:248:ILE:C	3:B:248:ILE:CD1	2.85	0.44
2:F:1909:DT:H1'	2:F:1910:DC:H5'	1.99	0.44
3:B:109:LEU:HB3	7:B:667:HOH:O	2.17	0.44
3:B:133:LEU:O	3:B:137:LYS:HA	2.18	0.44
3:B:297:SER:HB2	7:B:1134:HOH:O	2.17	0.44
3:A:3:VAL:HG13	7:A:1159:HOH:O	2.16	0.44
3:A:133:LEU:O	3:A:137:LYS:HA	2.18	0.44
3:B:142:VAL:HB	3:B:163:ILE:HG13	1.99	0.44
6:B:501:DGT:O3B	6:B:501:DGT:H5'A	2.17	0.44
3:A:157:MET:HE1	3:A:164:LYS:CE	2.48	0.43
7:D:1045:HOH:O	3:A:242:ARG:NH1	2.51	0.43
3:B:105:ASP:OD2	6:B:501:DGT:H5'	2.18	0.43
3:B:5:PHE:CD2	3:B:152:LYS:HA	2.53	0.43
3:A:163:ILE:O	3:A:163:ILE:HG23	2.18	0.43
3:B:217:ILE:HD12	3:B:221:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1912:DT:C2'	2:F:1913:DT:H72	2.47	0.43
3:A:197:LEU:HD22	3:A:212:LYS:HE2	2.00	0.43
3:A:280:ILE:CG2	3:A:305:GLY:HA3	2.48	0.43
3:B:116:ARG:HH11	3:B:116:ARG:HB3	1.83	0.43
3:B:46:ALA:HB1	3:B:50:ALA:HB3	2.00	0.43
1:E:1812:DT:C2'	1:E:1813:DOC:C5'	2.89	0.43
3:A:116:ARG:CD	7:A:1183:HOH:O	2.67	0.43
3:A:157:MET:HB2	3:A:157:MET:HE3	1.84	0.43
3:A:158:ALA:HB1	7:A:584:HOH:O	2.18	0.43
3:B:221:LYS:NZ	7:B:1061:HOH:O	2.52	0.43
3:A:118:TYR:CE2	3:A:167:ASP:HA	2.53	0.43
2:D:1904:DT:H2'	2:D:1904:DT:H6	1.30	0.43
3:B:116:ARG:HB3	3:B:116:ARG:CZ	2.48	0.43
3:B:238:ARG:HD3	7:B:665:HOH:O	2.19	0.43
3:B:329:LYS:HE2	7:B:807:HOH:O	2.19	0.43
3:A:155:ALA:CA	7:A:516:HOH:O	2.54	0.43
3:B:44:ALA:HB1	3:B:76:MET:HE2	1.99	0.43
3:A:140:VAL:N	7:A:673:HOH:O	2.52	0.42
3:A:242:ARG:NH1	3:A:242:ARG:CG	2.81	0.42
3:A:245:ILE:HD11	3:A:279:ARG:CZ	2.48	0.42
3:A:280:ILE:O	3:A:340:PHE:HA	2.19	0.42
3:B:198:GLY:HA2	7:B:932:HOH:O	2.19	0.42
3:B:209:GLU:HA	7:B:1191:HOH:O	2.19	0.42
3:B:11:PHE:N	7:B:648:HOH:O	2.52	0.42
3:B:301:THR:HG22	3:B:302:PHE:N	2.35	0.42
3:B:25:GLY:O	3:B:49:GLU:HG2	2.19	0.42
2:D:1904:DT:C5	3:A:293:LEU:HD11	2.54	0.42
1:E:1804:DG:H2''	1:E:1805:DG:OP2	2.20	0.42
3:A:137:LYS:HG2	7:A:1167:HOH:O	2.19	0.42
3:A:181:ALA:CB	3:A:195:LYS:NZ	2.82	0.42
3:B:255:SER:OG	3:B:256:ARG:N	2.52	0.42
3:A:259:GLU:O	3:A:263:PRO:HD3	2.19	0.42
3:B:224:TYR:CZ	3:B:228:LEU:HD11	2.55	0.42
3:B:242:ARG:NH1	3:B:242:ARG:HG3	2.28	0.42
3:B:314:GLU:O	3:B:318:LEU:HG	2.19	0.42
1:E:1812:DT:H1'	1:E:1813:DOC:H5'	2.01	0.42
3:A:20:ASN:HB3	3:A:23:LEU:HD12	2.01	0.42
3:B:194:LEU:C	3:B:196:LYS:N	2.73	0.42
3:B:258:LEU:O	3:B:262:LYS:HG3	2.20	0.42
3:B:287:VAL:HG22	7:B:1134:HOH:O	2.20	0.42
7:F:1053:HOH:O	3:B:220:ALA:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5:PHE:CD2	3:A:152:LYS:HA	2.54	0.42
2:D:1906:DG:H5'	3:A:32:VAL:HG11	2.00	0.42
3:B:270:GLU:OE2	3:B:308:LYS:HD3	2.20	0.42
3:A:100:GLU:HA	7:A:734:HOH:O	2.18	0.42
3:A:188:ASN:N	3:A:188:ASN:ND2	2.67	0.42
3:A:47:ASN:ND2	7:A:980:HOH:O	2.53	0.42
3:B:323:LEU:CD1	7:B:1184:HOH:O	2.67	0.42
1:E:1813:DOC:H3'2	7:B:788:HOH:O	2.19	0.42
3:A:197:LEU:HA	3:A:197:LEU:HD23	1.76	0.41
3:B:203:VAL:HG13	3:B:204:ASP:N	2.35	0.41
3:B:277:ASP:O	3:B:278:LYS:HB2	2.20	0.41
3:B:78:LYS:CG	7:B:1176:HOH:O	2.63	0.41
2:D:1903:DT:H1'	2:D:1904:DT:H5'	2.01	0.41
1:E:1802:DG:H1'	1:E:1803:DG:C8	2.55	0.41
3:A:181:ALA:CB	3:A:195:LYS:CE	2.92	0.41
3:A:202:LEU:C	7:A:1193:HOH:O	2.58	0.41
3:A:163:ILE:CG1	7:A:625:HOH:O	2.66	0.41
7:D:1147:HOH:O	3:A:221:LYS:NZ	2.41	0.41
3:B:209:GLU:HA	7:B:622:HOH:O	2.20	0.41
1:E:1806:DA:H2''	1:E:1807:DA:H8	1.85	0.41
3:A:44:ALA:HB1	3:A:76:MET:HE2	2.02	0.41
3:A:77:ARG:NH1	7:A:1218:HOH:O	2.52	0.41
7:F:529:HOH:O	3:B:293:LEU:HD22	2.19	0.41
2:F:1908:DA:C2	2:F:1909:DT:C2	3.08	0.41
3:A:247:ARG:C	7:A:1106:HOH:O	2.57	0.41
2:F:1902:DT:C3'	2:F:1903:DT:C4'	2.97	0.41
3:A:203:VAL:HG13	3:A:204:ASP:N	2.35	0.41
3:B:306:ILE:HG23	3:B:310:THR:HB	2.03	0.41
3:B:280:ILE:HB	3:B:341:ILE:HD12	2.02	0.41
2:D:1905:DT:H2'	7:D:747:HOH:O	2.21	0.41
3:A:286:VAL:HG23	3:A:318:LEU:HD12	2.03	0.41
3:A:294:ASP:C	7:A:1125:HOH:O	2.58	0.41
3:B:39:ASP:CB	7:B:1092:HOH:O	2.63	0.41
2:F:1903:DT:H2'	2:F:1904:DT:H2'	2.03	0.41
2:F:1904:DT:C1'	2:F:1905:DT:OP2	2.64	0.41
2:F:1912:DT:H2''	2:F:1913:DT:H72	2.03	0.41
3:A:295:ILE:HG12	7:A:1125:HOH:O	2.19	0.41
3:A:298:ARG:O	3:A:318:LEU:HD13	2.20	0.41
3:A:60:PRO:CD	7:A:879:HOH:O	2.68	0.41
3:A:53:PHE:O	3:A:67:ILE:HG21	2.21	0.41
3:A:55:VAL:HA	3:A:59:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:59:ILE:O	3:A:59:ILE:HG13	2.20	0.41
2:F:1903:DT:C2'	2:F:1904:DT:C5'	2.64	0.41
2:F:1912:DT:H2''	2:F:1913:DT:C7	2.50	0.41
3:A:10:TYR:HD1	3:A:13:ALA:HB3	1.86	0.41
3:A:189:ILE:HG22	3:A:190:THR:N	2.36	0.41
3:A:46:ALA:HB1	3:A:50:ALA:HB3	2.03	0.41
7:E:1076:HOH:O	3:B:187:GLY:HA3	2.20	0.41
3:B:194:LEU:C	3:B:196:LYS:H	2.25	0.41
3:A:193:LYS:HG3	7:A:1035:HOH:O	2.20	0.40
3:B:189:ILE:HG22	3:B:190:THR:N	2.36	0.40
1:E:1813:DOC:O2	7:E:928:HOH:O	2.21	0.40
3:B:172:LYS:HD2	7:B:982:HOH:O	2.21	0.40
3:B:208:ILE:HD11	3:B:212:LYS:HD3	2.03	0.40
3:B:266:PHE:CD1	3:B:312:TYR:CE1	3.09	0.40
3:B:51:ARG:HH22	6:B:501:DGT:PG	2.42	0.40
3:A:331:ARG:HG2	7:A:542:HOH:O	2.21	0.40
6:A:401:DGT:O1B	7:A:797:HOH:O	2.22	0.40
3:B:323:LEU:HD11	7:B:1184:HOH:O	2.21	0.40
2:D:1908:DA:OP2	3:A:336:ARG:NH2	2.46	0.40
2:F:1906:DG:H2''	2:F:1907:DA:OP2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	339/341 (99%)	309 (91%)	25 (7%)	5 (2%)	10	34
3	B	339/341 (99%)	310 (91%)	26 (8%)	3 (1%)	17	48
All	All	678/682 (99%)	619 (91%)	51 (8%)	8 (1%)	13	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	195	LYS
3	B	10	TYR
3	A	10	TYR
3	A	113	ASP
3	A	277	ASP
3	B	277	ASP
3	B	293	LEU
3	A	163	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	300/300 (100%)	290 (97%)	10 (3%)	38	72
3	B	300/300 (100%)	293 (98%)	7 (2%)	50	80
All	All	600/600 (100%)	583 (97%)	17 (3%)	43	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	79	GLU
3	A	145	SER
3	A	189	ILE
3	A	200	ASN
3	A	216	MET
3	A	234	ASN
3	A	248	ILE
3	A	297	SER
3	A	323	LEU
3	A	336	ARG
3	B	166	ILE
3	B	189	ILE
3	B	234	ASN
3	B	248	ILE
3	B	294	ASP
3	B	323	LEU

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Mol	Chain	Res	Type
3	B	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	188	ASN
3	A	200	ASN
3	A	304	HIS
3	B	14	GLN
3	B	188	ASN
3	B	234	ASN
3	B	285	HIS
3	B	304	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
1	DOC	C	1813	1,2	14,19,20	0.84	0	13,26,29	1.50	2 (15%)
1	DOC	E	1813	1,2	14,19,20	0.97	1 (7%)	13,26,29	1.25	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
1	DOC	C	1813	1,2	-	0/4/18/19	0/2/2/2
1	DOC	E	1813	1,2	-	1/4/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1813	DOC	C6-C5	-2.35	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1813	DOC	C2-N3-C4	3.73	120.12	116.34
1	E	1813	DOC	C2-N3-C4	3.68	120.07	116.34
1	C	1813	DOC	O4'-C4'-C5'	2.94	114.35	109.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	1813	DOC	O4'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1813	DOC	3	0
1	E	1813	DOC	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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	$\# Z > 2$
6	DGT	B	501	5,4	26,33,33	2.93	10 (38%)	32,52,52	3.42	19 (59%)
6	DGT	A	401	5,4	26,33,33	2.54	10 (38%)	32,52,52	2.71	14 (43%)

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
6	DGT	B	501	5,4	-	6/18/34/34	0/3/3/3
6	DGT	A	401	5,4	-	7/18/34/34	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	DGT	C6-N1	8.70	1.48	1.33
6	B	501	DGT	C6-N1	7.99	1.47	1.33
6	B	501	DGT	C8-N7	-7.41	1.21	1.34
6	B	501	DGT	C2-N1	4.68	1.43	1.35
6	A	401	DGT	C4-N3	4.02	1.41	1.35
6	B	501	DGT	O3'-C3'	-3.91	1.35	1.43
6	B	501	DGT	C4-N3	3.75	1.41	1.35
6	A	401	DGT	C2-N1	3.74	1.42	1.35
6	B	501	DGT	PG-O3G	3.56	1.62	1.50
6	A	401	DGT	PG-O3G	3.45	1.61	1.50
6	A	401	DGT	PB-O1B	-3.09	1.40	1.55
6	A	401	DGT	O5'-C5'	-2.77	1.34	1.44
6	A	401	DGT	PG-O1G	-2.75	1.44	1.54
6	B	501	DGT	C2'-C1'	-2.61	1.45	1.52
6	B	501	DGT	O4'-C4'	-2.58	1.39	1.45
6	A	401	DGT	C6-C5	2.52	1.45	1.41
6	B	501	DGT	PB-O1B	-2.29	1.44	1.55
6	A	401	DGT	C8-N7	-2.28	1.30	1.34
6	A	401	DGT	O3'-C3'	-2.19	1.38	1.43
6	B	501	DGT	O5'-C5'	2.04	1.52	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	DGT	C2'-C1'-N9	9.99	137.31	114.27
6	A	401	DGT	C6-C5-C4	-6.98	114.14	120.80
6	B	501	DGT	C5-C6-N1	-6.57	114.45	123.43
6	B	501	DGT	C4-C5-N7	6.44	116.11	109.40
6	A	401	DGT	N3-C2-N1	-5.66	119.67	127.22
6	B	501	DGT	C6-N1-C2	5.46	124.61	115.93
6	A	401	DGT	O5'-C5'-C4'	4.85	125.68	108.99
6	B	501	DGT	N3-C2-N1	-4.70	120.95	127.22
6	A	401	DGT	C6-N1-C2	4.49	123.07	115.93
6	A	401	DGT	C5-C6-N1	-4.47	117.31	123.43
6	B	501	DGT	O1G-PG-O3B	-3.92	91.48	104.64
6	A	401	DGT	C4-C5-N7	3.89	113.45	109.40
6	A	401	DGT	O2G-PG-O1G	3.79	122.11	107.64
6	B	501	DGT	O2G-PG-O1G	3.73	121.90	107.64
6	B	501	DGT	C2'-C3'-C4'	3.30	109.63	102.76
6	B	501	DGT	C6-C5-C4	-3.23	117.72	120.80
6	A	401	DGT	O1B-PB-O2B	3.12	127.65	112.24
6	B	501	DGT	PA-O5'-C5'	3.06	139.62	121.68
6	B	501	DGT	N2-C2-N1	2.98	121.89	117.25
6	B	501	DGT	C5'-C4'-C3'	2.95	132.10	114.74
6	B	501	DGT	O2G-PG-O3B	2.90	114.35	104.64
6	A	401	DGT	C5'-C4'-C3'	-2.80	98.31	114.74
6	B	501	DGT	O1B-PB-O2B	2.67	125.42	112.24
6	B	501	DGT	C2-N3-C4	-2.57	112.42	115.36
6	B	501	DGT	O1A-PA-O5'	2.51	119.42	107.75
6	A	401	DGT	O1G-PG-O3B	-2.46	96.39	104.64
6	B	501	DGT	O4'-C1'-C2'	2.41	110.81	106.25
6	A	401	DGT	O1A-PA-O2A	2.31	123.66	112.24
6	A	401	DGT	O3'-C3'-C2'	2.23	118.88	110.90
6	A	401	DGT	N2-C2-N1	2.21	120.69	117.25
6	B	501	DGT	O4'-C4'-C3'	-2.10	100.77	105.67
6	A	401	DGT	PA-O3A-PB	-2.09	125.65	132.83
6	B	501	DGT	O4'-C4'-C5'	-2.08	102.53	109.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	DGT	PB-O3B-PG-O1G
6	A	401	DGT	C3'-C4'-C5'-O5'
6	B	501	DGT	PB-O3A-PA-O5'
6	B	501	DGT	C5'-O5'-PA-O3A
6	B	501	DGT	O4'-C4'-C5'-O5'

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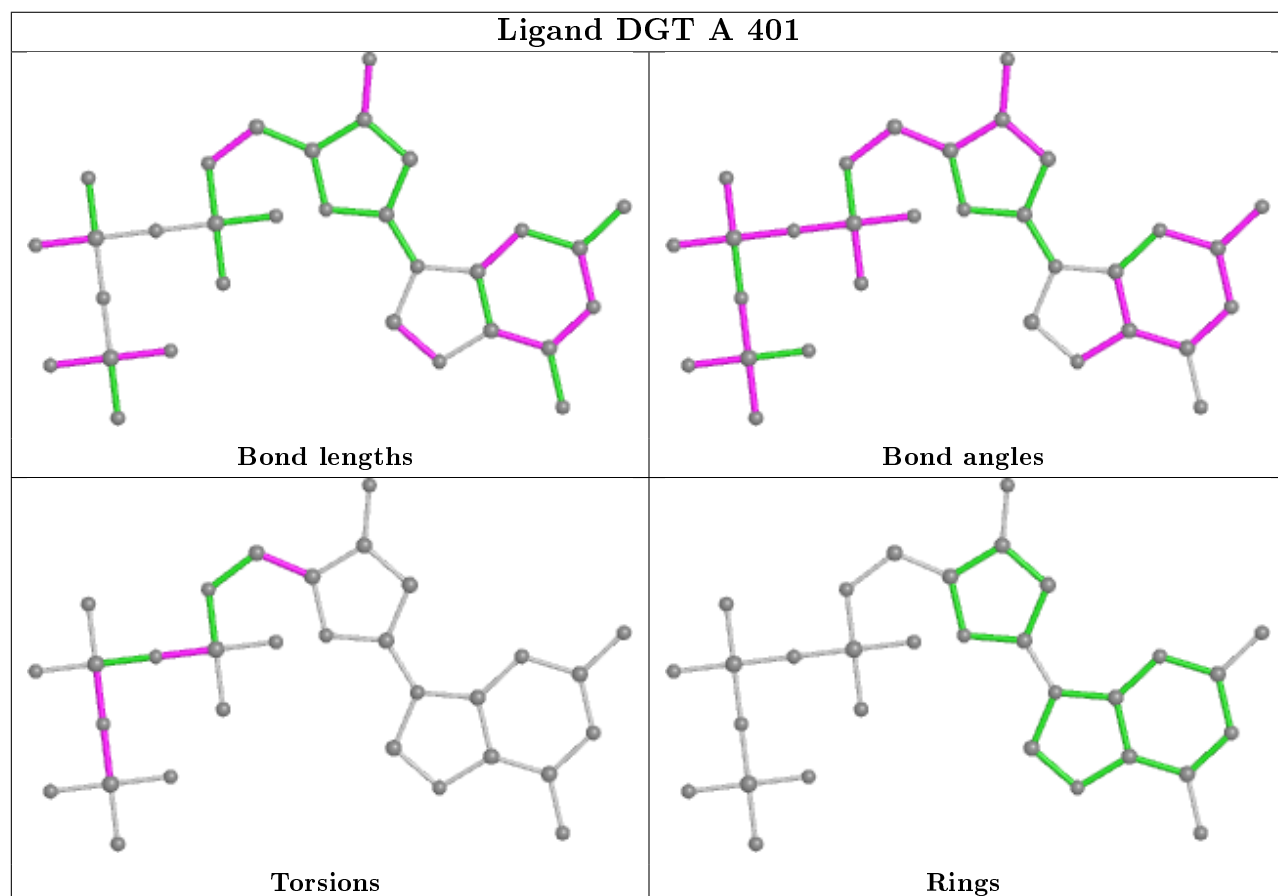
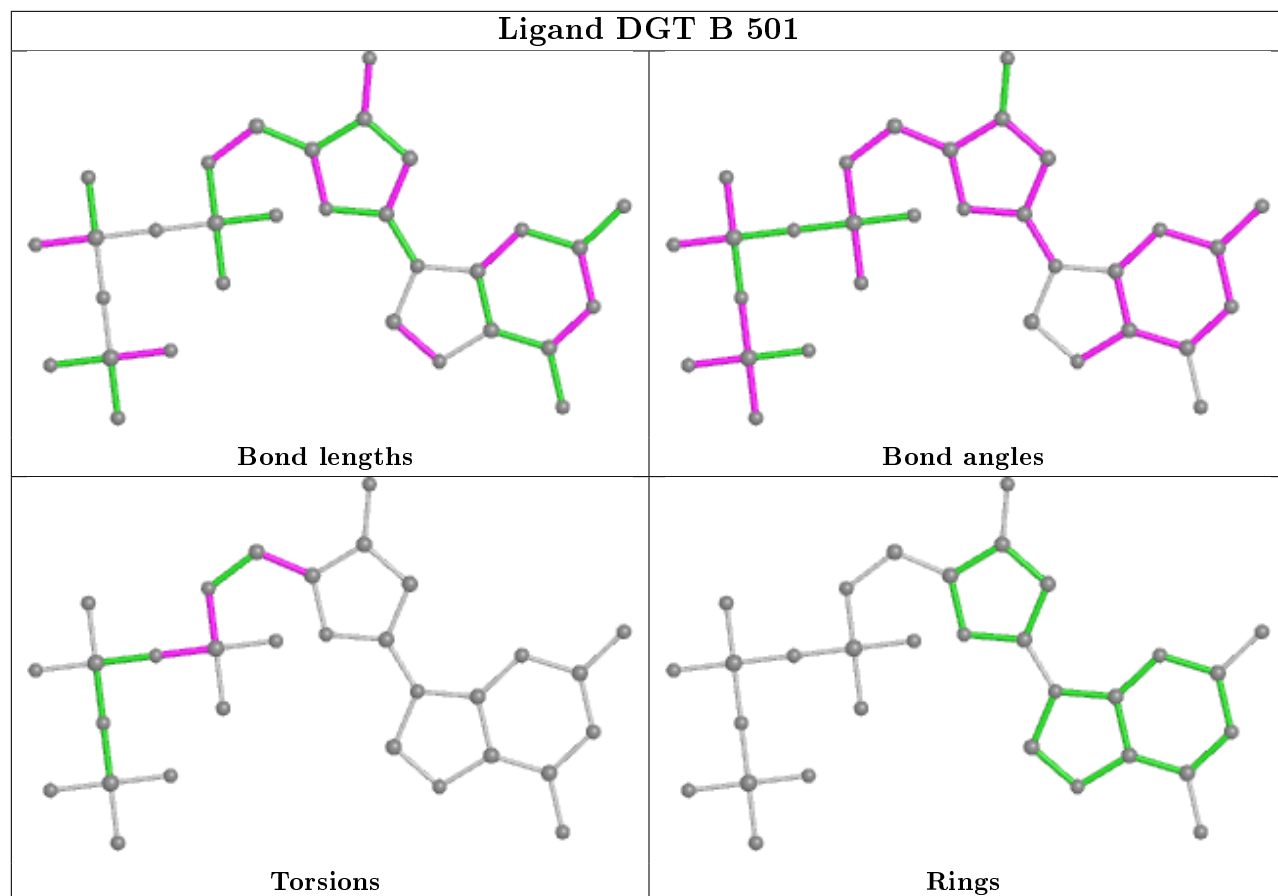
Mol	Chain	Res	Type	Atoms
6	B	501	DGT	C3'-C4'-C5'-O5'
6	A	401	DGT	O4'-C4'-C5'-O5'
6	A	401	DGT	PB-O3A-PA-O5'
6	A	401	DGT	PG-O3B-PB-O1B
6	B	501	DGT	C5'-O5'-PA-O1A
6	B	501	DGT	C5'-O5'-PA-O2A
6	A	401	DGT	PG-O3B-PB-O2B
6	A	401	DGT	PB-O3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	DGT	4	0
6	A	401	DGT	11	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	12/13 (92%)	-0.01	0 100 100	46, 69, 81, 92	0
1	E	12/13 (92%)	-0.12	0 100 100	52, 72, 80, 81	0
2	D	17/17 (100%)	0.22	2 (11%) 4 3	53, 77, 173, 176	0
2	F	17/17 (100%)	0.17	1 (5%) 22 18	44, 73, 160, 160	0
3	A	341/341 (100%)	-0.39	2 (0%) 89 89	25, 54, 85, 111	0
3	B	341/341 (100%)	-0.41	0 100 100	27, 54, 84, 106	0
All	All	740/742 (99%)	-0.36	5 (0%) 87 87	25, 55, 88, 176	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	195	LYS	2.9
2	F	1902	DT	2.8
3	A	116	ARG	2.4
2	D	1903	DT	2.3
2	D	1904	DT	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	DOC	C	1813	18/19	0.77	0.42	99,110,118,119	0
1	DOC	E	1813	18/19	0.92	0.26	66,93,113,113	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

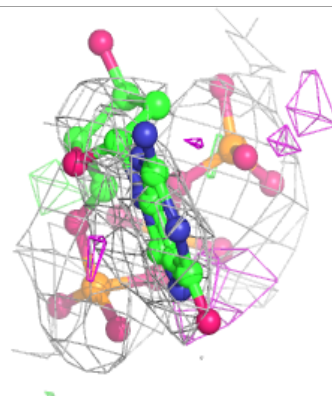
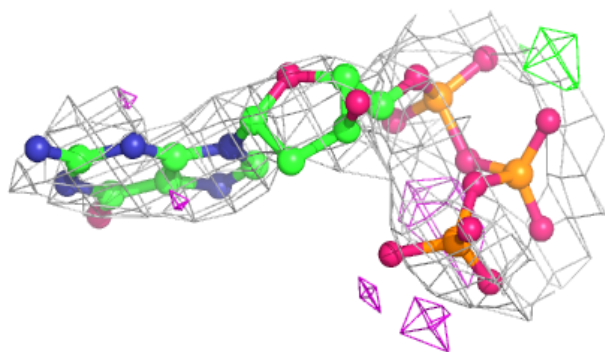
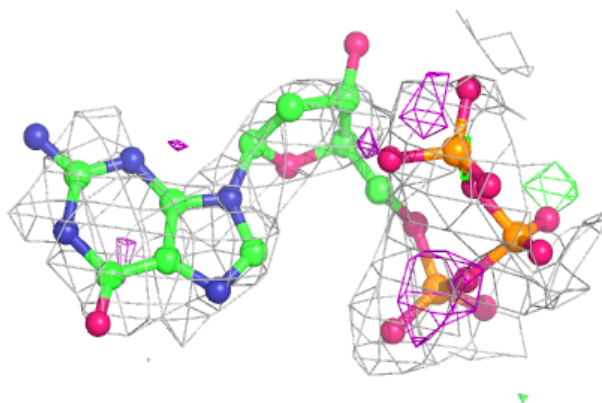
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	403	1/1	0.88	0.22	49,49,49,49	0
6	DGT	A	401	31/31	0.92	0.25	114,121,128,129	0
4	CA	A	402	1/1	0.93	0.18	59,59,59,59	0
5	MG	B	408	1/1	0.93	0.13	32,32,32,32	0
6	DGT	B	501	31/31	0.93	0.26	108,131,134,134	0
4	CA	B	402	1/1	0.98	0.11	47,47,47,47	0
5	MG	A	404	1/1	0.98	0.07	33,33,33,33	0
5	MG	B	407	1/1	0.98	0.08	43,43,43,43	0
5	MG	B	404	1/1	0.99	0.10	38,38,38,38	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.

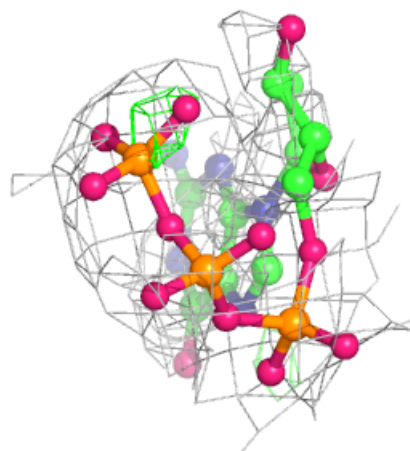
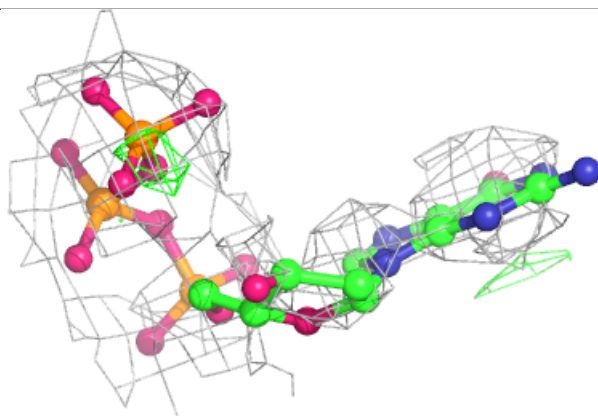
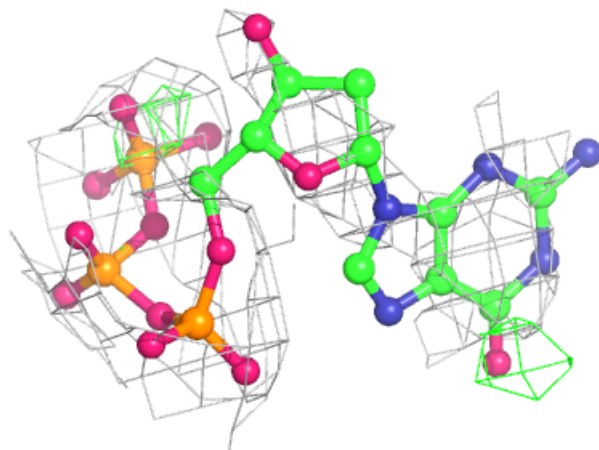
Electron density around DGT A 401:

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



Electron density around DGT B 501:

$2mF_o-DF_c$ (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.