



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:30 PM BST

PDB ID : 2W7P
Title : Structure and Activity of Bypass Synthesis by Human DNA Polymerase Kappa
Opposite the 7,8-Dihydro-8-oxodeoxyguanosine Adduct
Authors : Irimia, A.; Egli, M.
Deposited on : 2008-12-23
Resolution : 3.71 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 : 2.13.1
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) : 2.13.1

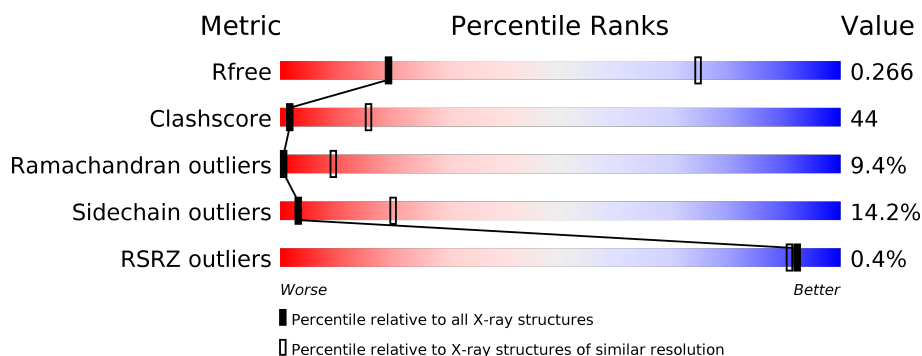
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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	A	508	<div> <div>30%</div> <div>44%</div> <div>10%</div> <div>15%</div> </div>
1	B	508	<div> <div>27%</div> <div>43%</div> <div>14%</div> <div>•</div> <div>15%</div> </div>
2	E	13	<div> <div>8%</div> <div>77%</div> <div>15%</div> </div>
2	P	13	<div> <div>100%</div> </div>
3	F	18	<div> <div>50%</div> <div>28%</div> <div>6%</div> <div>17%</div> </div>
3	T	18	<div> <div>28%</div> <div>67%</div> <div>6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA POLYMERASE KAPPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	1
			3461	2181	613	646	21			
1	B	431	Total	C	N	O	S	0	0	1
			3452	2175	611	645	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			229	109	47	63	10			
2	P	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 3 is a DNA chain called 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	15	Total	C	N	O	P	0	0	0
			298	143	52	89	14			
3	T	17	Total	C	N	O	P	0	0	0
			336	161	58	101	16			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

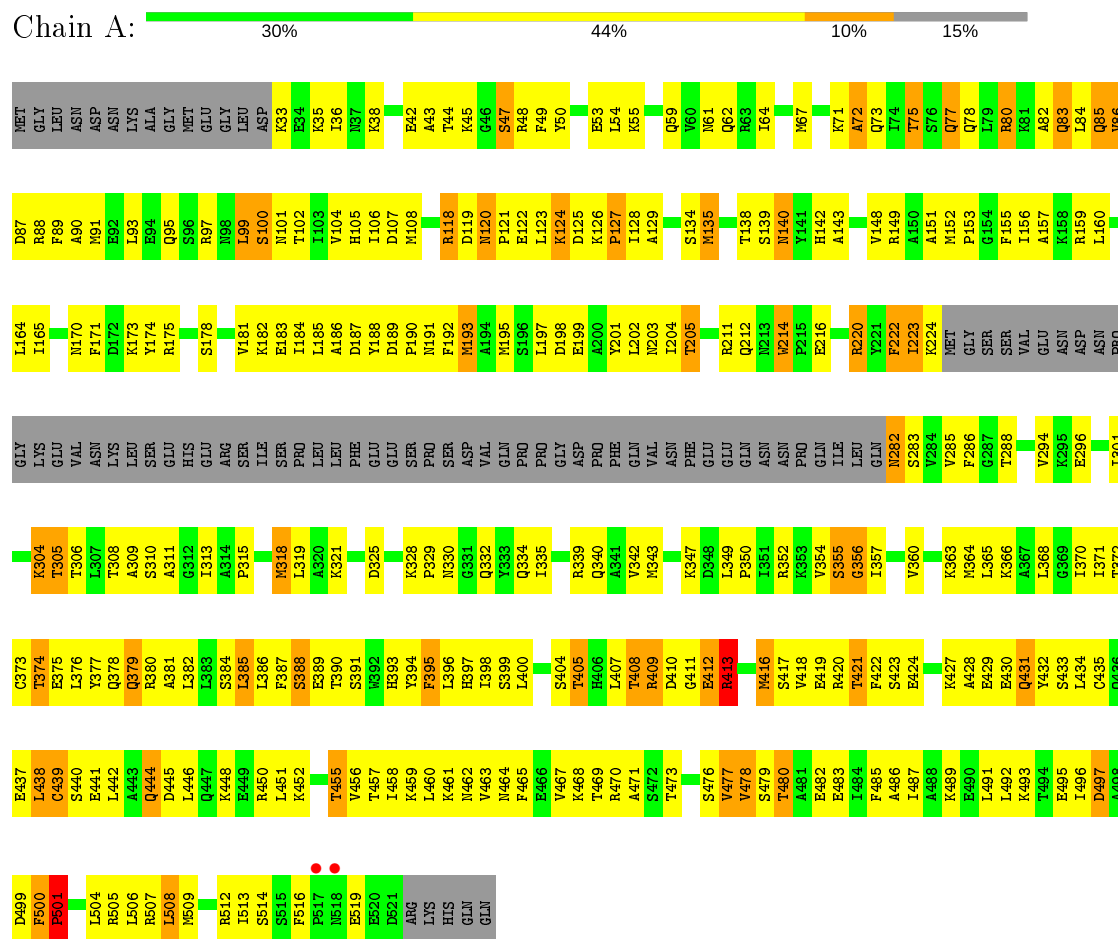
- Molecule 6 is water.

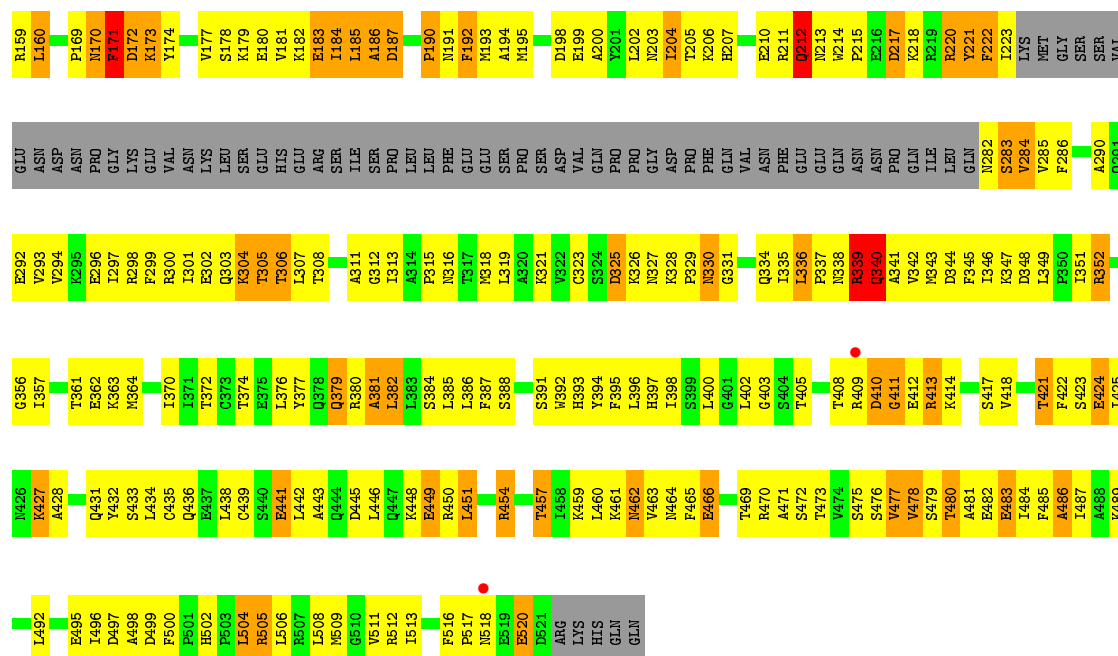
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	F	1	Total	O	0	0
			1	1		
6	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

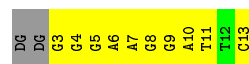
• Molecule 1: DNA POLYMERASE KAPPA





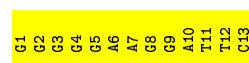
- Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3'

Chain E: 8% 77% 15%



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

Chain P: 100%



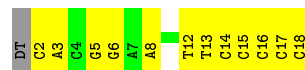
- Molecule 3: 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP* TP*CP*CP*CP*CP*C)-3'

Chain F: 50% 28% 6% 17%



- Molecule 3: 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP* TP*CP*CP*CP*CP*C)-3'

Chain T: 28% 67% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	167.83Å 220.85Å 119.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.65 – 3.71 44.65 – 3.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.65-3.71) 97.0 (44.65-3.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.236 , 0.273 0.225 , 0.266	Depositor DCC
R_{free} test set	1112 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, CA, DTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/3514	0.77	3/4722 (0.1%)
1	B	0.43	0/3505	0.69	0/4711
2	E	0.69	0/258	0.62	0/398
2	P	0.71	0/308	0.67	0/476
3	F	0.65	0/305	0.64	0/464
3	T	0.71	0/347	0.68	0/528
All	All	0.50	0/8237	0.72	3/11299 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	PHE	C-N-CD	-21.67	72.93	120.60
1	A	500	PHE	C-N-CA	12.24	173.41	122.00
1	A	501	PRO	CA-N-CD	-5.14	104.30	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	282	ASN	Peptide
2	P	12	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	A	3461	0	3544	321	0
1	B	3452	0	3531	333	0
2	E	229	0	125	15	0
2	P	273	0	147	16	0
3	F	298	0	170	11	0
3	T	336	0	192	20	0
4	A	30	0	12	1	0
4	B	30	0	12	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	10	0	0	4	0
6	F	1	0	0	0	0
6	T	1	0	0	0	0
All	All	8125	0	7733	696	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 44.

All (696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:THR:HG23	1:A:483:GLU:HG2	1.22	1.14
1:B:75:THR:HG23	1:B:78:GLN:HB2	1.29	1.12
3:F:6:DG:H2"	3:F:7:DA:H5"	1.28	1.12
1:B:457:THR:HG23	1:B:471:ALA:HB2	1.34	1.08
1:B:480:THR:HG23	1:B:483:GLU:HG3	1.34	1.03
2:E:3:DG:H2"	2:E:4:DG:H5"	1.40	1.02
1:B:449:GLU:O	1:B:451:LEU:HD13	1.64	0.98
3:T:13:DT:H2"	3:T:14:DC:H5"	1.46	0.97
1:A:485:PHE:CE1	1:A:489:LYS:HB3	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:PHE:O	1:B:489:LYS:HB2	1.66	0.95
1:A:457:THR:HG23	1:A:471:ALA:HB2	1.48	0.95
1:B:301:ILE:O	1:B:305:THR:HG22	1.65	0.95
3:T:12:DT:H2''	3:T:13:DT:H5''	1.50	0.93
1:A:84:LEU:HB2	1:B:95:GLN:HE22	1.34	0.92
1:B:357:ILE:HD12	1:B:361:THR:HG21	1.50	0.91
1:B:204:ILE:O	1:B:204:ILE:HG13	1.69	0.91
1:B:99:LEU:HD13	1:B:337:PRO:O	1.69	0.91
3:F:6:DG:C2'	3:F:7:DA:H5''	2.00	0.90
1:B:305:THR:HG23	1:B:307:LEU:H	1.35	0.89
1:B:283:SER:O	1:B:284:VAL:HG22	1.73	0.88
1:A:75:THR:HG23	1:A:78:GLN:OE1	1.75	0.87
3:F:6:DG:H2''	3:F:7:DA:C5'	2.04	0.87
1:B:461:LYS:HB3	1:B:508:LEU:HB3	1.56	0.85
1:A:170:ASN:HD22	1:A:173:LYS:HB2	1.40	0.84
1:A:170:ASN:ND2	1:A:173:LYS:HB2	1.92	0.84
1:B:106:ILE:O	1:B:199:GLU:HA	1.77	0.84
1:A:452:LYS:HB3	1:A:477:VAL:O	1.77	0.83
1:A:452:LYS:HG2	1:A:479:SER:HB2	1.58	0.83
1:B:417:SER:HB3	1:B:512:ARG:HG3	1.60	0.82
1:B:480:THR:CG2	1:B:483:GLU:HG3	2.09	0.82
1:A:480:THR:CG2	1:A:483:GLU:HG2	2.05	0.82
1:A:461:LYS:HB2	1:A:508:LEU:HD12	1.62	0.81
1:A:385:LEU:O	1:A:386:LEU:HD23	1.80	0.81
3:T:13:DT:H2''	3:T:14:DC:C5'	2.11	0.80
1:B:120:ASN:H	1:B:121:PRO:HD3	1.44	0.80
1:B:123:LEU:C	1:B:125:ASP:H	1.84	0.80
3:T:13:DT:C2'	3:T:14:DC:H5''	2.12	0.80
1:B:33:LYS:HD2	1:B:33:LYS:O	1.81	0.79
1:B:207:HIS:NE2	1:B:211:ARG:HD3	1.97	0.79
1:A:366:LYS:HD3	1:A:371:ILE:HD11	1.66	0.79
1:A:508:LEU:HD22	1:A:509:MET:N	1.98	0.79
1:B:504:LEU:HD12	1:B:504:LEU:H	1.49	0.78
1:B:119:ASP:O	1:B:120:ASN:HB2	1.80	0.77
1:A:478:VAL:HG13	1:A:483:GLU:CB	2.15	0.77
1:B:325:ASP:HA	1:B:328:LYS:HB2	1.67	0.77
1:A:463:VAL:HG23	1:A:505:ARG:O	1.85	0.77
1:A:178:SER:O	1:A:181:VAL:HG12	1.85	0.76
1:A:223:ILE:HG23	1:A:224:LYS:H	1.48	0.76
1:A:343:MET:HE2	6:A:2005:HOH:O	1.85	0.76
1:B:111:PHE:O	1:B:115:VAL:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:O	1:B:177:VAL:HG23	1.86	0.76
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.51	0.75
1:B:39:ILE:HG21	1:B:160:LEU:HD12	1.68	0.75
1:A:97:ARG:HG2	1:A:99:LEU:CD1	2.17	0.75
1:B:313:ILE:HB	1:B:334:GLN:HG3	1.69	0.75
1:B:221:TYR:CD2	1:B:300:ARG:HD2	2.22	0.75
1:A:84:LEU:HB2	1:B:95:GLN:NE2	2.02	0.74
1:A:101:ASN:HA	1:A:205:THR:HG21	1.69	0.74
1:A:44:THR:O	1:A:47:SER:HB3	1.88	0.74
1:B:408:THR:HG22	1:B:409:ARG:H	1.54	0.73
1:A:370:ILE:HD13	1:A:376:LEU:HD12	1.69	0.73
1:B:305:THR:HG23	1:B:307:LEU:N	2.03	0.73
1:B:500:PHE:C	1:B:502:HIS:H	1.92	0.73
1:A:171:PHE:HA	1:A:174:TYR:HD1	1.53	0.73
1:B:319:LEU:HD11	1:B:342:VAL:HG13	1.69	0.72
1:A:377:TYR:HB2	1:A:399:SER:HB3	1.70	0.72
1:A:120:ASN:C	1:A:120:ASN:HD22	1.92	0.72
1:A:118:ARG:HD2	1:A:119:ASP:OD2	1.90	0.72
2:P:2:DG:H2''	2:P:3:DG:OP2	1.88	0.72
1:A:356:GLY:HA3	1:A:394:TYR:OH	1.90	0.72
1:B:480:THR:O	1:B:483:GLU:HB2	1.90	0.71
1:B:107:ASP:HA	1:B:198:ASP:O	1.90	0.71
1:B:460:LEU:HD22	1:B:506:LEU:HD21	1.71	0.71
1:B:504:LEU:HD22	1:B:506:LEU:HD11	1.72	0.71
1:B:508:LEU:HD13	1:B:509:MET:N	2.04	0.71
1:A:478:VAL:HG13	1:A:483:GLU:HB3	1.70	0.71
1:B:497:ASP:O	1:B:499:ASP:N	2.22	0.71
1:A:61:ASN:HD21	1:A:363:LYS:NZ	1.87	0.71
1:A:379:GLN:NE2	1:B:340:GLN:HG3	2.06	0.71
1:A:347:LYS:O	1:A:374:THR:HB	1.89	0.71
1:A:357:ILE:HD11	1:A:394:TYR:HE2	1.53	0.71
1:A:413:ARG:NH2	1:A:416:MET:HG2	2.06	0.70
1:A:138:THR:HG22	1:A:139:SER:H	1.57	0.69
1:A:459:LYS:HG3	1:A:469:THR:HG22	1.74	0.69
1:A:430:GLU:O	1:A:433:SER:HB2	1.92	0.69
1:A:313:ILE:HB	1:A:334:GLN:HG3	1.73	0.69
2:E:3:DG:C2'	2:E:4:DG:H5''	2.20	0.69
1:A:97:ARG:HG2	1:A:99:LEU:HD13	1.74	0.69
1:B:428:ALA:O	1:B:432:TYR:HD1	1.76	0.69
1:A:102:THR:H	1:A:205:THR:HG23	1.58	0.69
1:A:384:SER:C	1:A:385:LEU:HD23	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD22	1:A:509:MET:H	1.58	0.69
1:A:491:LEU:H	1:A:491:LEU:HD12	1.58	0.69
1:B:38:LYS:O	1:B:42:GLU:HB2	1.92	0.69
1:B:478:VAL:HG13	1:B:483:GLU:OE2	1.93	0.69
3:T:12:DT:C2'	3:T:13:DT:H5''	2.23	0.68
1:B:138:THR:HG22	1:B:139:SER:N	2.09	0.68
1:A:343:MET:CE	6:A:2005:HOH:O	2.40	0.68
1:B:169:PRO:C	1:B:171:PHE:H	1.97	0.68
1:B:293:VAL:O	1:B:297:ILE:HG13	1.94	0.68
1:B:516:PHE:HB3	1:B:517:PRO:HD2	1.75	0.68
1:A:417:SER:HB3	1:A:512:ARG:CG	2.23	0.68
1:B:417:SER:HB3	1:B:512:ARG:CG	2.24	0.68
1:A:140:ASN:H	1:A:140:ASN:HD22	1.42	0.68
1:A:418:VAL:CG2	6:A:2010:HOH:O	2.43	0.67
1:A:460:LEU:HD22	1:A:506:LEU:HD21	1.75	0.67
1:A:420:ARG:NH1	1:A:434:LEU:HD11	2.09	0.67
1:A:467:VAL:HG12	1:A:468:LYS:N	2.09	0.67
1:B:190:PRO:HG2	1:B:191:ASN:H	1.59	0.67
1:B:477:VAL:HG12	1:B:477:VAL:O	1.95	0.67
3:F:2:DC:H2'	3:F:2:DC:O2	1.94	0.67
1:A:155:PHE:CE1	1:A:156:ILE:HG13	2.29	0.67
1:B:117:MET:SD	1:B:128:ILE:HD11	2.34	0.67
1:B:298:ARG:NH1	1:B:331:GLY:HA2	2.10	0.67
1:A:308:THR:HG21	1:A:330:ASN:HD22	1.60	0.66
1:A:497:ASP:HA	1:A:500:PHE:HB2	1.77	0.66
1:A:50:TYR:CE1	1:A:54:LEU:HD21	2.30	0.66
1:A:465:PHE:HE2	1:A:507:ARG:CZ	2.09	0.66
1:B:334:GLN:HG2	1:B:335:ILE:H	1.58	0.66
1:A:193:MET:HB2	1:A:409:ARG:HG2	1.76	0.66
1:A:514:SER:HA	1:A:516:PHE:HE1	1.61	0.66
1:B:334:GLN:HG2	1:B:335:ILE:N	2.10	0.66
1:B:352:ARG:HG3	1:B:352:ARG:HH11	1.59	0.66
1:B:296:GLU:O	1:B:299:PHE:HB3	1.96	0.66
1:B:462:ASN:HB3	1:B:464:ASN:OD1	1.96	0.65
1:A:101:ASN:HB2	1:A:405:THR:HG22	1.78	0.65
1:A:55:LYS:HE3	1:A:59:GLN:HB2	1.78	0.65
1:B:476:SER:O	1:B:477:VAL:HB	1.96	0.65
1:B:290:ALA:O	1:B:293:VAL:HG22	1.97	0.65
1:A:462:ASN:HD21	1:A:464:ASN:HB2	1.62	0.65
1:A:80:ARG:HB3	1:A:80:ARG:HH11	1.62	0.65
1:B:170:ASN:O	1:B:172:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:12:DT:H2"	3:T:13:DT:C5'	2.25	0.64
1:A:514:SER:HA	1:A:516:PHE:CE1	2.33	0.64
1:B:126:LYS:HB3	1:B:127:PRO:HD2	1.79	0.64
1:B:408:THR:HG22	1:B:409:ARG:N	2.13	0.64
1:A:310:SER:HB2	1:A:328:LYS:NZ	2.13	0.64
1:A:308:THR:CG2	1:A:330:ASN:HD22	2.10	0.64
1:B:427:LYS:H	1:B:427:LYS:HD2	1.63	0.64
1:A:462:ASN:ND2	1:A:464:ASN:HB2	2.13	0.63
1:B:313:ILE:HD12	1:B:313:ILE:N	2.12	0.63
1:B:192:PHE:HD1	1:B:193:MET:N	1.95	0.63
1:A:462:ASN:ND2	1:A:464:ASN:H	1.96	0.63
1:B:442:LEU:O	1:B:442:LEU:HD12	1.99	0.63
3:T:2:DC:H2"	3:T:3:DA:O5'	1.98	0.63
1:B:185:LEU:O	1:B:187:ASP:N	2.32	0.62
1:B:217:ASP:O	1:B:220:ARG:HB2	1.99	0.62
1:B:86:VAL:HG11	1:B:380:ARG:HB2	1.81	0.62
1:B:492:LEU:HD12	1:B:492:LEU:O	1.99	0.62
1:B:508:LEU:HD13	1:B:508:LEU:C	2.19	0.62
1:A:49:PHE:HA	1:A:465:PHE:CE1	2.34	0.62
1:B:336:LEU:N	1:B:336:LEU:HD23	2.14	0.62
2:E:8:DG:H1'	2:E:9:DG:H5"	1.82	0.62
1:A:478:VAL:HG13	1:A:483:GLU:HB2	1.81	0.61
1:A:95:GLN:NE2	1:B:84:LEU:HB2	2.15	0.61
1:A:171:PHE:HA	1:A:174:TYR:CD1	2.33	0.61
1:B:47:SER:C	1:B:49:PHE:H	2.04	0.61
1:A:106:ILE:CD1	1:A:185:LEU:HD21	2.30	0.61
1:A:500:PHE:CG	1:A:501:PRO:HD3	2.34	0.61
3:F:5:8OG:H2'	3:F:6:DG:O5'	2.00	0.61
2:E:4:DG:H2"	2:E:5:DG:C8	2.35	0.61
1:A:286:PHE:CE2	1:A:296:GLU:HA	2.35	0.61
1:A:119:ASP:OD1	1:A:173:LYS:HD3	2.01	0.60
1:A:310:SER:HB2	1:A:328:LYS:HZ1	1.66	0.60
1:B:54:LEU:HD13	1:B:57:GLU:OE1	2.02	0.60
1:A:75:THR:C	1:A:77:GLN:H	2.05	0.60
1:B:463:VAL:HG12	1:B:463:VAL:O	2.02	0.60
1:B:312:GLY:HA3	1:B:323:CYS:HB2	1.82	0.60
1:A:465:PHE:CE2	1:A:507:ARG:CZ	2.85	0.60
1:B:120:ASN:N	1:B:121:PRO:HD3	2.16	0.60
1:B:302:GLU:O	1:B:306:THR:HA	2.00	0.60
1:A:134:SER:O	1:A:153:PRO:HA	2.01	0.60
2:E:7:DA:H5'	2:E:7:DA:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG22	1:A:139:SER:N	2.17	0.59
1:A:140:ASN:HD21	1:A:143:ALA:HB2	1.66	0.59
1:B:347:LYS:O	1:B:348:ASP:HB2	2.01	0.59
3:T:17:DC:H2''	3:T:18:DC:H5''	1.84	0.59
1:A:55:LYS:CE	1:A:59:GLN:HB2	2.32	0.59
1:A:372:THR:OG1	1:A:374:THR:HG22	2.03	0.59
1:A:395:PHE:HD2	1:A:395:PHE:H	1.50	0.59
1:A:123:LEU:HD22	1:A:128:ILE:HG21	1.83	0.59
1:A:223:ILE:HG23	1:A:224:LYS:N	2.17	0.59
1:A:121:PRO:O	1:A:123:LEU:N	2.35	0.59
1:A:368:LEU:N	1:A:368:LEU:HD12	2.18	0.59
1:A:108:MET:HA	1:A:309:ALA:HB2	1.84	0.59
1:A:123:LEU:HD22	1:A:128:ILE:CG2	2.32	0.58
1:B:120:ASN:H	1:B:121:PRO:CD	2.15	0.58
1:B:194:ALA:HA	1:B:200:ALA:CB	2.32	0.58
1:B:454:ARG:HH22	1:B:475:SER:HA	1.68	0.58
2:P:10:DA:H1'	2:P:11:DT:H5'	1.84	0.58
1:B:417:SER:N	3:F:8:DA:OP2	2.37	0.58
1:B:508:LEU:HD22	1:B:509:MET:H	1.69	0.58
1:A:164:LEU:HD12	1:A:165:ILE:H	1.69	0.58
1:A:446:LEU:CD1	1:A:513:ILE:HG21	2.33	0.58
1:B:121:PRO:O	1:B:122:GLU:HB3	2.02	0.58
1:A:97:ARG:HG2	1:A:99:LEU:HD11	1.85	0.58
1:B:459:LYS:O	1:B:509:MET:HA	2.04	0.58
1:B:129:ALA:HB1	1:B:136:LEU:HD21	1.85	0.58
1:B:414:LYS:HD2	1:B:414:LYS:N	2.17	0.58
1:B:222:PHE:O	1:B:223:ILE:HG23	2.04	0.57
1:B:463:VAL:HG23	1:B:505:ARG:O	2.04	0.57
1:B:63:ARG:NH2	1:B:364:MET:HE1	2.19	0.57
1:B:500:PHE:C	1:B:502:HIS:N	2.58	0.57
1:A:376:LEU:HD11	1:A:395:PHE:HD1	1.69	0.57
1:B:505:ARG:HD3	1:B:505:ARG:N	2.19	0.57
1:A:360:VAL:HG21	2:P:10:DA:H3'	1.85	0.57
1:B:48:ARG:HD2	1:B:463:VAL:HG12	1.87	0.57
3:F:6:DG:C3'	3:F:7:DA:H5''	2.31	0.57
1:A:339:ARG:HH11	1:A:339:ARG:HG2	1.70	0.57
1:B:129:ALA:HB1	1:B:136:LEU:CD2	2.34	0.57
1:A:310:SER:OG	1:A:328:LYS:HG3	2.04	0.57
1:B:182:LYS:O	1:B:185:LEU:HB2	2.04	0.57
1:B:105:HIS:CE1	1:B:321:LYS:HD2	2.40	0.56
1:B:417:SER:HB3	1:B:512:ARG:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:14:DC:H2"	3:T:15:DC:C6	2.39	0.56
1:B:97:ARG:NH1	1:B:339:ARG:NH1	2.53	0.56
1:A:452:LYS:HG2	1:A:479:SER:CB	2.32	0.56
1:A:455:THR:OG1	1:A:473:THR:HA	2.05	0.56
1:A:192:PHE:O	1:A:193:MET:O	2.24	0.56
1:B:422:PHE:CE1	1:B:425:ILE:HD12	2.41	0.56
1:B:339:ARG:HG3	1:B:339:ARG:NH1	2.19	0.56
1:A:71:LYS:O	1:A:73:GLN:N	2.39	0.56
3:F:4:DC:H6	3:F:4:DC:H5'	1.70	0.56
1:A:412:GLU:O	1:A:413:ARG:HB3	2.05	0.56
1:B:47:SER:C	1:B:49:PHE:N	2.56	0.56
1:B:505:ARG:H	1:B:505:ARG:HD3	1.71	0.56
1:B:128:ILE:O	1:B:129:ALA:HB2	2.07	0.55
1:A:101:ASN:N	1:A:101:ASN:HD22	2.02	0.55
1:A:365:LEU:HD21	1:A:395:PHE:HE1	1.70	0.55
1:B:286:PHE:CD1	1:B:296:GLU:HG3	2.42	0.55
1:A:368:LEU:HD12	1:A:368:LEU:H	1.71	0.55
1:B:74:ILE:HG22	1:B:78:GLN:HB3	1.88	0.55
1:B:292:GLU:HA	1:B:292:GLU:OE2	2.06	0.55
1:A:220:ARG:NH1	1:A:220:ARG:HB2	2.21	0.55
1:A:378:GLN:NE2	1:B:343:MET:HE2	2.22	0.55
1:B:220:ARG:HG2	1:B:221:TYR:N	2.22	0.55
1:B:497:ASP:C	1:B:499:ASP:H	2.09	0.55
1:B:382:LEU:HD22	1:B:386:LEU:HG	1.89	0.55
1:A:170:ASN:H	1:A:174:TYR:HE1	1.55	0.55
1:A:485:PHE:HE1	1:A:489:LYS:HB3	1.64	0.55
1:B:476:SER:O	1:B:477:VAL:CB	2.54	0.55
1:A:413:ARG:HH21	1:A:416:MET:HG2	1.72	0.55
1:A:48:ARG:NH1	1:A:463:VAL:HG12	2.21	0.55
1:B:431:GLN:HE22	1:B:504:LEU:HD11	1.72	0.55
1:A:452:LYS:HE2	1:A:479:SER:CB	2.37	0.54
1:A:55:LYS:O	1:A:55:LYS:HD2	2.07	0.54
1:A:64:ILE:HD11	1:A:364:MET:HA	1.88	0.54
1:B:305:THR:HG23	1:B:306:THR:N	2.21	0.54
2:E:9:DG:H2"	2:E:10:DA:H8	1.71	0.54
1:A:463:VAL:HG12	1:A:463:VAL:O	2.06	0.54
1:B:212:GLN:CD	1:B:213:ASN:H	2.11	0.54
1:B:421:THR:HG23	1:B:508:LEU:HB2	1.90	0.54
3:T:15:DC:H2"	3:T:16:DC:OP2	2.06	0.54
1:A:128:ILE:C	1:A:128:ILE:HD12	2.27	0.54
1:B:210:GLU:C	1:B:212:GLN:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HD2	1:A:357:ILE:O	2.08	0.54
1:B:179:LYS:HA	1:B:182:LYS:HB2	1.88	0.54
1:A:223:ILE:HG12	1:A:224:LYS:N	2.23	0.54
1:A:216:GLU:HG3	1:A:285:VAL:HG21	1.88	0.54
1:B:308:THR:HB	1:B:330:ASN:HD22	1.73	0.54
1:A:334:GLN:HG2	1:A:335:ILE:N	2.23	0.54
1:A:467:VAL:HG12	1:A:468:LYS:H	1.72	0.54
1:B:351:ILE:HD11	1:B:376:LEU:HD22	1.90	0.54
1:B:180:GLU:O	1:B:183:GLU:HB2	2.08	0.54
1:A:38:LYS:HG2	1:A:38:LYS:O	2.08	0.54
1:B:123:LEU:C	1:B:125:ASP:N	2.55	0.54
1:A:83:GLN:HG2	1:A:381:ALA:HB2	1.90	0.54
1:B:427:LYS:O	1:B:431:GLN:HG3	2.08	0.54
1:B:435:CYS:O	1:B:438:LEU:HB2	2.08	0.54
3:F:5:8OG:C2'	3:F:6:DG:O5'	2.56	0.54
1:A:437:GLU:O	1:A:440:SER:HB3	2.08	0.53
1:A:461:LYS:HB3	1:A:508:LEU:HB3	1.89	0.53
2:E:7:DA:H2''	2:E:8:DG:O5'	2.08	0.53
1:A:408:THR:O	1:A:409:ARG:HB2	2.07	0.53
1:B:192:PHE:CD1	1:B:193:MET:N	2.77	0.53
1:B:210:GLU:O	1:B:212:GLN:HG3	2.09	0.53
1:B:316:ASN:HD21	1:B:319:LEU:H	1.57	0.53
1:B:377:TYR:O	1:B:380:ARG:HG2	2.09	0.53
2:E:10:DA:H2''	2:E:11:DT:H5'	1.88	0.53
1:A:360:VAL:CG2	2:P:10:DA:H3'	2.38	0.53
1:B:424:GLU:HG3	1:B:425:ILE:N	2.24	0.53
1:B:436:GLN:HB2	1:B:485:PHE:CE2	2.44	0.53
1:A:77:GLN:NE2	1:A:78:GLN:N	2.57	0.53
1:B:179:LYS:O	1:B:183:GLU:HG3	2.09	0.53
1:B:210:GLU:O	1:B:214:TRP:CD1	2.62	0.53
1:B:204:ILE:HD12	1:B:293:VAL:HG21	1.90	0.53
1:B:329:PRO:O	1:B:330:ASN:HB3	2.09	0.52
1:B:107:ASP:HB3	1:B:328:LYS:HE2	1.91	0.52
1:B:212:GLN:NE2	1:B:213:ASN:H	2.06	0.52
1:B:328:LYS:C	1:B:330:ASN:H	2.11	0.52
1:A:378:GLN:NE2	1:B:343:MET:CE	2.73	0.52
1:A:186:ALA:C	1:A:188:TYR:H	2.12	0.52
1:B:115:VAL:O	1:B:119:ASP:HB2	2.09	0.52
1:B:117:MET:HE2	1:B:118:ARG:HG2	1.90	0.52
1:B:464:ASN:ND2	1:B:466:GLU:HG3	2.24	0.52
1:B:97:ARG:HH21	1:B:402:LEU:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:HH11	1:A:450:ARG:HG3	1.74	0.52
1:B:122:GLU:O	1:B:125:ASP:HB2	2.09	0.52
1:B:138:THR:CG2	1:B:139:SER:N	2.73	0.52
1:B:496:ILE:HG12	1:B:504:LEU:HD21	1.91	0.52
1:A:197:LEU:N	1:A:197:LEU:HD12	2.24	0.52
1:A:417:SER:HB3	1:A:512:ARG:CB	2.39	0.52
1:B:351:ILE:CD1	1:B:376:LEU:HD22	2.39	0.52
1:B:412:GLU:O	1:B:413:ARG:HB2	2.10	0.52
1:A:120:ASN:C	1:A:120:ASN:ND2	2.62	0.52
1:B:480:THR:C	1:B:483:GLU:HB2	2.30	0.52
1:A:203:ASN:HB2	1:A:407:LEU:CD1	2.40	0.52
1:A:420:ARG:HH11	1:A:434:LEU:HD11	1.75	0.52
1:A:61:ASN:HD21	1:A:363:LYS:HZ2	1.56	0.52
1:B:454:ARG:NH2	1:B:475:SER:HA	2.25	0.52
1:A:127:PRO:O	1:A:164:LEU:HD12	2.10	0.52
1:A:318:MET:HE3	1:A:354:VAL:HG13	1.92	0.52
1:A:491:LEU:H	1:A:491:LEU:CD1	2.23	0.52
1:A:71:LYS:HD3	1:A:72:ALA:N	2.25	0.52
1:B:304:LYS:HG3	1:B:304:LYS:O	2.09	0.52
1:B:327:ASN:C	1:B:329:PRO:HD2	2.30	0.52
1:B:343:MET:HE3	1:B:346:ILE:CG2	2.41	0.51
1:B:396:LEU:O	1:B:396:LEU:HD12	2.08	0.51
1:B:220:ARG:HG2	1:B:221:TYR:H	1.74	0.51
1:A:49:PHE:HA	1:A:465:PHE:CD1	2.45	0.51
1:B:97:ARG:HH12	1:B:339:ARG:NH1	2.08	0.51
1:A:418:VAL:HG22	6:A:2010:HOH:O	2.07	0.51
1:B:114:ALA:O	1:B:307:LEU:HD21	2.10	0.51
1:B:121:PRO:O	1:B:122:GLU:CB	2.59	0.51
1:B:316:ASN:HD22	1:B:403:GLY:HA3	1.76	0.51
1:A:128:ILE:HD11	1:A:140:ASN:HB3	1.92	0.51
1:A:83:GLN:NE2	1:A:87:ASP:OD2	2.44	0.51
1:B:116:GLU:O	1:B:120:ASN:HB3	2.10	0.51
1:B:192:PHE:C	1:B:192:PHE:CD1	2.84	0.51
1:A:101:ASN:O	1:A:315:PRO:HA	2.10	0.51
1:A:106:ILE:HD12	1:A:185:LEU:HD21	1.92	0.51
1:A:305:THR:O	1:A:306:THR:HB	2.10	0.51
1:A:182:LYS:O	1:A:185:LEU:N	2.43	0.51
1:B:116:GLU:OE1	1:B:170:ASN:HB2	2.10	0.51
1:B:431:GLN:HE22	1:B:504:LEU:CD1	2.23	0.51
1:A:222:PHE:HA	1:A:282:ASN:O	2.11	0.51
1:A:321:LYS:HG2	1:A:355:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:O	1:A:125:ASP:N	2.44	0.50
1:A:75:THR:C	1:A:77:GLN:N	2.63	0.50
1:B:303:GLN:C	1:B:305:THR:H	2.14	0.50
1:B:132:SER:OG	1:B:133:MET:N	2.44	0.50
1:A:446:LEU:HD11	1:A:513:ILE:HG21	1.92	0.50
1:B:218:LYS:C	1:B:220:ARG:H	2.14	0.50
1:B:138:THR:HG22	1:B:139:SER:H	1.74	0.50
1:B:285:VAL:HG22	1:B:286:PHE:H	1.75	0.50
1:B:376:LEU:HG	1:B:376:LEU:O	2.12	0.50
1:B:470:ARG:HG3	1:B:495:GLU:OE2	2.12	0.50
1:A:223:ILE:O	1:A:224:LYS:CB	2.60	0.50
1:A:382:LEU:O	1:A:382:LEU:HD23	2.12	0.50
1:B:123:LEU:O	1:B:125:ASP:N	2.44	0.50
1:B:39:ILE:CG2	1:B:160:LEU:HD12	2.39	0.50
1:A:62:GLN:C	1:A:64:ILE:N	2.64	0.50
1:A:419:GLU:HB2	1:A:508:LEU:HD21	1.93	0.50
1:B:329:PRO:O	1:B:330:ASN:CB	2.59	0.50
1:B:414:LYS:CD	1:B:414:LYS:N	2.74	0.50
1:A:305:THR:O	1:A:306:THR:CB	2.60	0.49
1:B:326:LYS:HG3	1:B:327:ASN:ND2	2.27	0.49
1:B:33:LYS:C	1:B:35:LYS:H	2.15	0.49
1:B:33:LYS:O	1:B:36:ILE:HG13	2.12	0.49
1:A:44:THR:HG22	1:A:50:TYR:HB2	1.93	0.49
1:A:328:LYS:CG	1:A:329:PRO:HA	2.41	0.49
1:A:89:PHE:CE1	1:A:93:LEU:HD21	2.48	0.49
1:B:120:ASN:O	1:B:121:PRO:O	2.29	0.49
1:B:220:ARG:HD2	1:B:222:PHE:CE2	2.48	0.49
1:A:140:ASN:N	1:A:140:ASN:HD22	2.06	0.49
1:B:94:GLU:CD	1:B:339:ARG:HH12	2.15	0.49
1:A:155:PHE:CG	3:T:3:DA:OP1	2.66	0.49
1:A:203:ASN:C	1:A:205:THR:H	2.16	0.49
1:A:417:SER:HB3	1:A:512:ARG:HA	1.93	0.49
1:B:202:LEU:HD23	1:B:202:LEU:N	2.27	0.49
1:B:53:GLU:O	1:B:57:GLU:HG3	2.13	0.49
1:A:118:ARG:CD	1:A:119:ASP:OD2	2.58	0.49
1:A:507:ARG:HH11	1:A:507:ARG:HG2	1.77	0.49
2:E:5:DG:H2''	2:E:6:DA:C8	2.47	0.49
2:P:1:DG:H2''	2:P:2:DG:O5'	2.13	0.49
1:A:102:THR:H	1:A:205:THR:CG2	2.23	0.49
1:B:128:ILE:O	1:B:129:ALA:CB	2.61	0.49
1:B:316:ASN:ND2	1:B:319:LEU:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:HB3	1:B:391:SER:HB2	1.94	0.49
1:B:472:SER:HB3	1:B:487:ILE:HG21	1.95	0.49
1:A:121:PRO:O	1:A:124:LYS:HB2	2.13	0.49
1:A:108:MET:HA	1:A:309:ALA:CB	2.43	0.49
1:A:49:PHE:CA	1:A:465:PHE:CE1	2.96	0.49
1:B:286:PHE:CE1	1:B:296:GLU:HG3	2.47	0.49
1:B:445:ASP:HA	1:B:448:LYS:HE3	1.95	0.49
1:B:340:GLN:O	1:B:344:ASP:OD2	2.30	0.48
1:A:417:SER:HB3	1:A:512:ARG:HG3	1.94	0.48
1:A:423:SER:O	1:A:424:GLU:C	2.49	0.48
1:B:205:THR:HG23	1:B:206:LYS:N	2.29	0.48
1:B:184:ILE:HG23	1:B:300:ARG:CZ	2.43	0.48
1:B:408:THR:CG2	1:B:409:ARG:H	2.19	0.48
1:A:203:ASN:HB2	1:A:407:LEU:HD11	1.95	0.48
1:B:220:ARG:HD2	1:B:222:PHE:HE2	1.78	0.48
1:A:387:PHE:O	1:A:388:SER:O	2.31	0.48
1:B:126:LYS:CB	1:B:127:PRO:HD2	2.44	0.48
1:B:305:THR:CG2	1:B:306:THR:N	2.76	0.48
1:B:387:PHE:CD2	1:B:395:PHE:HE1	2.31	0.48
2:E:7:DA:C8	2:E:7:DA:H5'	2.48	0.48
1:A:452:LYS:CG	1:A:479:SER:HB2	2.35	0.48
1:B:194:ALA:HA	1:B:200:ALA:HB1	1.95	0.48
1:B:305:THR:CG2	1:B:307:LEU:H	2.17	0.48
1:B:71:LYS:O	1:B:73:GLN:N	2.41	0.48
1:A:483:GLU:O	1:A:486:ALA:HB3	2.13	0.48
1:B:159:ARG:HH11	1:B:159:ARG:HG3	1.78	0.48
1:B:410:ASP:O	1:B:411:GLY:O	2.31	0.48
1:A:127:PRO:HB3	1:A:142:HIS:CE1	2.49	0.48
1:A:357:ILE:CD1	1:A:394:TYR:HE2	2.25	0.48
1:B:285:VAL:HG22	1:B:286:PHE:N	2.29	0.48
1:B:330:ASN:CG	1:B:330:ASN:O	2.51	0.48
1:A:491:LEU:HD12	1:A:491:LEU:N	2.25	0.48
1:B:352:ARG:HG3	1:B:352:ARG:NH1	2.27	0.48
1:A:508:LEU:C	1:A:508:LEU:HD13	2.35	0.47
1:B:35:LYS:O	1:B:38:LYS:HB3	2.14	0.47
1:B:464:ASN:HD21	1:B:466:GLU:HG3	1.79	0.47
1:B:286:PHE:HD1	1:B:296:GLU:OE2	1.96	0.47
1:B:328:LYS:N	1:B:329:PRO:HD2	2.29	0.47
1:B:328:LYS:C	1:B:330:ASN:N	2.66	0.47
1:B:68:MET:O	1:B:71:LYS:HB3	2.15	0.47
2:E:4:DG:C2'	2:E:5:DG:C8	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HG3	1:A:329:PRO:HA	1.96	0.47
3:T:12:DT:C4	3:T:13:DT:O4	2.67	0.47
1:A:467:VAL:CG1	1:A:468:LYS:N	2.76	0.47
1:B:394:TYR:CE2	1:B:398:ILE:HD11	2.50	0.47
1:B:40:ILE:O	1:B:42:GLU:N	2.46	0.47
1:B:109:ASP:O	1:B:111:PHE:N	2.43	0.47
1:B:141:TYR:OH	1:B:329:PRO:HA	2.14	0.47
4:B:1521:DTP:O4'	2:E:13:DC:H2"	2.14	0.47
1:B:179:LYS:HA	1:B:182:LYS:HD2	1.95	0.47
1:B:424:GLU:OE1	1:B:505:ARG:HB3	2.15	0.47
1:A:43:ALA:HB1	1:A:159:ARG:HH12	1.79	0.47
1:A:382:LEU:HD21	1:A:386:LEU:HD11	1.97	0.47
1:B:185:LEU:O	1:B:186:ALA:C	2.53	0.47
1:B:308:THR:HB	1:B:330:ASN:ND2	2.29	0.47
1:B:347:LYS:HG2	1:B:348:ASP:OD1	2.14	0.47
1:B:135:MET:HG3	3:F:5:8OG:O4'	2.14	0.47
1:A:421:THR:HG23	1:A:508:LEU:HB2	1.96	0.47
1:A:446:LEU:HD12	1:A:513:ILE:HG21	1.97	0.47
1:A:123:LEU:O	1:A:126:LYS:HG2	2.14	0.47
1:A:427:LYS:HB3	1:A:430:GLU:HG3	1.97	0.47
1:A:492:LEU:O	1:A:496:ILE:HG13	2.14	0.47
1:B:305:THR:O	1:B:306:THR:CB	2.62	0.47
1:B:315:PRO:O	1:B:405:THR:HG22	2.15	0.47
1:B:461:LYS:HG3	1:B:465:PHE:HA	1.96	0.47
1:A:121:PRO:C	1:A:123:LEU:N	2.68	0.47
1:B:146:PHE:O	1:B:160:LEU:HD23	2.14	0.47
1:B:338:ASN:ND2	1:B:341:ALA:N	2.63	0.47
1:B:417:SER:O	1:B:418:VAL:HG23	2.15	0.47
1:B:77:GLN:OE1	1:B:77:GLN:C	2.52	0.47
1:A:318:MET:CE	1:A:354:VAL:HG13	2.45	0.46
1:A:438:LEU:O	1:A:441:GLU:N	2.48	0.46
1:B:120:ASN:N	1:B:121:PRO:CD	2.76	0.46
1:B:313:ILE:CB	1:B:334:GLN:HG3	2.43	0.46
1:A:192:PHE:CD1	1:A:193:MET:N	2.83	0.46
1:A:349:LEU:HD22	1:A:373:CYS:SG	2.55	0.46
1:A:461:LYS:CB	1:A:508:LEU:HD12	2.39	0.46
1:A:294:VAL:HG12	1:A:332:GLN:OE1	2.14	0.46
1:A:395:PHE:CD2	1:A:395:PHE:N	2.83	0.46
1:A:427:LYS:O	1:A:431:GLN:NE2	2.49	0.46
1:B:306:THR:O	1:B:306:THR:HG22	2.15	0.46
1:B:517:PRO:O	1:B:520:GLU:OE2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:HD21	1:B:341:ALA:HB2	1.81	0.46
1:B:442:LEU:HD21	1:B:513:ILE:HG22	1.96	0.46
1:B:52:ASN:HB2	1:B:464:ASN:O	2.16	0.46
1:A:155:PHE:CD2	3:T:3:DA:OP1	2.68	0.46
1:A:477:VAL:O	1:A:478:VAL:O	2.33	0.46
1:B:119:ASP:O	1:B:120:ASN:CB	2.58	0.46
1:B:215:PRO:HD2	1:B:218:LYS:HD2	1.98	0.46
1:B:330:ASN:OD1	1:B:330:ASN:O	2.34	0.46
1:B:408:THR:HG21	1:B:410:ASP:OD2	2.16	0.46
2:P:2:DG:H1'	2:P:3:DG:O5'	2.16	0.46
1:B:485:PHE:O	1:B:489:LYS:CB	2.53	0.46
1:A:185:LEU:HD22	1:A:202:LEU:HD21	1.98	0.46
1:A:184:ILE:HD12	1:A:301:ILE:HG12	1.98	0.46
1:A:371:ILE:HB	1:A:375:GLU:OE2	2.16	0.46
1:A:387:PHE:O	1:A:388:SER:C	2.53	0.46
1:A:86:VAL:HG11	1:A:380:ARG:HB2	1.97	0.46
1:B:177:VAL:O	1:B:177:VAL:HG12	2.15	0.46
1:B:462:ASN:CB	1:B:464:ASN:OD1	2.64	0.46
1:B:504:LEU:HD12	1:B:504:LEU:N	2.25	0.46
1:A:507:ARG:NH1	1:A:507:ARG:HG2	2.32	0.45
1:B:384:SER:C	1:B:385:LEU:HD23	2.37	0.45
1:B:438:LEU:O	1:B:441:GLU:N	2.49	0.45
2:E:4:DG:H2'	2:E:5:DG:N7	2.31	0.45
1:A:339:ARG:HG2	1:A:339:ARG:NH1	2.29	0.45
1:A:38:LYS:O	1:A:42:GLU:HB2	2.17	0.45
1:B:50:TYR:CE1	1:B:54:LEU:HD21	2.51	0.45
2:P:6:DA:C6	2:P:7:DA:C6	3.04	0.45
1:A:211:ARG:O	1:A:212:GLN:C	2.54	0.45
1:A:463:VAL:CG1	1:A:463:VAL:O	2.63	0.45
1:B:105:HIS:NE2	1:B:321:LYS:HD2	2.31	0.45
1:B:83:GLN:NE2	1:B:381:ALA:HB2	2.31	0.45
1:A:135:MET:HE1	1:A:152:MET:C	2.37	0.45
1:A:155:PHE:CD1	1:A:156:ILE:N	2.85	0.45
1:B:36:ILE:CG2	1:B:160:LEU:HD21	2.47	0.45
1:A:438:LEU:O	1:A:439:CYS:C	2.53	0.45
1:A:487:ILE:HG22	1:A:491:LEU:HD11	1.97	0.45
1:B:169:PRO:C	1:B:171:PHE:N	2.68	0.45
1:B:207:HIS:C	1:B:207:HIS:CD2	2.90	0.45
1:B:356:GLY:HA3	1:B:394:TYR:OH	2.17	0.45
1:B:138:THR:CG2	1:B:139:SER:H	2.30	0.45
1:B:352:ARG:HD3	1:B:352:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:17:DC:H2''	3:T:18:DC:C5'	2.45	0.45
1:B:169:PRO:O	1:B:171:PHE:N	2.49	0.45
1:B:516:PHE:CD1	1:B:516:PHE:N	2.84	0.45
1:A:128:ILE:HD12	1:A:140:ASN:ND2	2.31	0.45
1:A:182:LYS:O	1:A:184:ILE:N	2.50	0.45
1:A:421:THR:OG1	3:T:6:DG:OP2	2.34	0.45
1:A:97:ARG:HD3	1:A:99:LEU:HD21	1.97	0.45
1:A:199:GLU:OE1	2:P:13:DC:H5''	2.17	0.45
2:P:8:DG:N2	3:T:12:DT:O2	2.49	0.45
1:A:67:MET:CE	1:A:368:LEU:HD11	2.47	0.45
1:B:338:ASN:ND2	1:B:341:ALA:H	2.15	0.45
1:B:478:VAL:CG1	1:B:483:GLU:HB3	2.47	0.45
1:B:497:ASP:C	1:B:499:ASP:N	2.69	0.45
1:A:100:SER:C	1:A:101:ASN:HD22	2.21	0.44
1:A:107:ASP:OD1	4:A:1521:DTP:O2B	2.35	0.44
1:A:170:ASN:HD22	1:A:173:LYS:CB	2.22	0.44
1:A:181:VAL:CG2	1:A:301:ILE:HD13	2.47	0.44
1:A:385:LEU:HD23	1:A:385:LEU:N	2.33	0.44
1:A:108:MET:SD	1:A:309:ALA:HB2	2.57	0.44
1:A:461:LYS:HE2	1:A:465:PHE:HD2	1.82	0.44
2:P:4:DG:H2''	2:P:5:DG:O5'	2.18	0.44
1:A:127:PRO:HB3	1:A:142:HIS:ND1	2.32	0.44
1:A:417:SER:O	1:A:418:VAL:HG23	2.17	0.44
1:A:442:LEU:O	1:A:446:LEU:HB2	2.17	0.44
1:A:473:THR:HG22	2:P:6:DA:OP1	2.17	0.44
1:B:136:LEU:HB2	1:B:152:MET:O	2.18	0.44
1:B:171:PHE:HA	1:B:174:TYR:CD1	2.51	0.44
1:B:210:GLU:C	1:B:212:GLN:N	2.70	0.44
1:B:425:ILE:CG2	1:B:431:GLN:HG2	2.48	0.44
1:A:223:ILE:CG2	1:A:282:ASN:HB3	2.48	0.44
1:A:99:LEU:N	1:A:99:LEU:CD1	2.80	0.44
1:B:47:SER:O	1:B:49:PHE:N	2.50	0.44
1:B:97:ARG:NH2	1:B:400:LEU:O	2.50	0.44
2:E:9:DG:C2'	2:E:10:DA:H8	2.30	0.44
1:A:413:ARG:NH2	3:T:8:DA:OP1	2.51	0.44
1:A:148:VAL:HG22	1:A:157:ALA:HB1	2.00	0.44
1:A:33:LYS:O	1:A:36:ILE:HG13	2.17	0.44
1:B:302:GLU:O	1:B:302:GLU:HG2	2.17	0.44
1:B:140:ASN:OD1	1:B:143:ALA:HB2	2.18	0.44
1:B:215:PRO:HD2	1:B:218:LYS:CG	2.48	0.44
1:A:170:ASN:C	1:A:174:TYR:HE1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:O	1:A:214:TRP:HB2	2.18	0.44
1:B:155:PHE:O	1:B:159:ARG:HG2	2.18	0.44
1:B:422:PHE:HD1	1:B:423:SER:O	2.01	0.44
2:P:6:DA:N6	2:P:7:DA:N6	2.65	0.44
1:A:354:VAL:HG11	1:A:398:ILE:HD13	1.99	0.44
1:B:127:PRO:HG3	1:B:142:HIS:O	2.17	0.44
1:A:197:LEU:N	1:A:197:LEU:CD1	2.81	0.43
1:A:102:THR:N	1:A:205:THR:HG23	2.30	0.43
1:B:499:ASP:O	1:B:500:PHE:HB2	2.18	0.43
1:B:83:GLN:HG3	1:B:83:GLN:O	2.17	0.43
1:A:77:GLN:HE21	1:A:78:GLN:N	2.16	0.43
1:B:328:LYS:O	1:B:330:ASN:N	2.51	0.43
1:A:393:HIS:O	1:A:397:HIS:CD2	2.71	0.43
1:B:178:SER:O	1:B:181:VAL:HG12	2.18	0.43
1:B:414:LYS:CD	1:B:414:LYS:H	2.31	0.43
1:A:140:ASN:HD21	1:A:143:ALA:CB	2.32	0.43
1:A:170:ASN:C	1:A:174:TYR:CE1	2.92	0.43
1:B:203:ASN:C	1:B:205:THR:H	2.21	0.43
1:A:140:ASN:ND2	1:A:143:ALA:CB	2.82	0.43
1:A:349:LEU:HA	1:A:350:PRO:HD3	1.84	0.43
1:A:446:LEU:CD2	1:A:446:LEU:O	2.67	0.43
1:A:500:PHE:CD2	1:A:501:PRO:N	2.87	0.43
1:B:103:ILE:CG2	1:B:104:VAL:N	2.81	0.43
1:B:149:ARG:O	1:B:150:ALA:O	2.36	0.43
1:B:207:HIS:CD2	1:B:207:HIS:O	2.72	0.43
1:B:316:ASN:ND2	1:B:318:MET:HB3	2.33	0.43
1:B:298:ARG:HH12	1:B:331:GLY:HA2	1.81	0.43
1:B:338:ASN:ND2	1:B:341:ALA:HB2	2.34	0.43
1:A:445:ASP:O	1:A:448:LYS:HE2	2.18	0.43
1:B:155:PHE:C	1:B:155:PHE:CD2	2.92	0.43
1:B:370:ILE:HD11	1:B:379:GLN:CB	2.49	0.43
1:B:408:THR:C	1:B:409:ARG:HG3	2.39	0.43
1:B:478:VAL:HG13	1:B:483:GLU:HB3	1.99	0.43
1:B:502:HIS:N	1:B:502:HIS:CD2	2.87	0.43
1:A:319:LEU:HD21	1:A:342:VAL:HG13	2.01	0.43
1:A:438:LEU:O	1:A:440:SER:N	2.52	0.43
1:A:75:THR:O	1:A:77:GLN:N	2.52	0.43
1:B:127:PRO:HA	1:B:143:ALA:HB2	2.00	0.43
1:B:107:ASP:OD2	1:B:198:ASP:OD2	2.37	0.43
1:B:442:LEU:C	1:B:442:LEU:HD12	2.37	0.43
1:B:504:LEU:O	1:B:504:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:O	1:A:83:GLN:C	2.57	0.43
1:A:128:ILE:HG22	1:A:165:ILE:HB	2.01	0.43
1:A:186:ALA:O	1:A:188:TYR:N	2.52	0.43
1:A:199:GLU:CD	2:P:13:DC:H5''	2.40	0.43
1:A:120:ASN:HA	1:A:121:PRO:HD2	1.80	0.42
1:A:377:TYR:CB	1:A:399:SER:HB3	2.45	0.42
1:B:103:ILE:HG22	1:B:104:VAL:N	2.34	0.42
1:B:343:MET:HA	1:B:346:ILE:HG22	2.01	0.42
1:A:174:TYR:O	1:A:175:ARG:C	2.57	0.42
1:A:108:MET:HB2	1:A:198:ASP:HB2	2.00	0.42
1:A:101:ASN:ND2	1:A:101:ASN:N	2.67	0.42
1:B:40:ILE:HG22	1:B:41:MET:N	2.34	0.42
3:T:17:DC:C2'	3:T:18:DC:H5''	2.47	0.42
1:A:128:ILE:HD12	1:A:140:ASN:HD22	1.83	0.42
1:A:64:ILE:CD1	1:A:364:MET:HA	2.47	0.42
1:A:463:VAL:HG23	1:A:505:ARG:C	2.40	0.42
1:B:115:VAL:HG22	1:B:307:LEU:HD11	2.00	0.42
1:B:221:TYR:CE2	1:B:300:ARG:NH1	2.88	0.42
1:B:424:GLU:HG3	1:B:425:ILE:H	1.83	0.42
1:A:328:LYS:HB2	1:A:328:LYS:HE2	1.78	0.42
1:A:456:VAL:O	1:A:471:ALA:HB1	2.19	0.42
1:A:82:ALA:O	1:A:85:GLN:N	2.53	0.42
1:B:313:ILE:CD1	1:B:313:ILE:N	2.82	0.42
1:B:349:LEU:HD23	1:B:349:LEU:C	2.40	0.42
1:B:424:GLU:O	1:B:425:ILE:HG13	2.18	0.42
1:B:508:LEU:HD22	1:B:509:MET:N	2.32	0.42
1:A:203:ASN:OD1	1:A:205:THR:OG1	2.38	0.42
1:A:349:LEU:HD23	1:A:349:LEU:O	2.20	0.42
1:A:354:VAL:HG11	1:A:398:ILE:CD1	2.50	0.42
1:A:77:GLN:NE2	1:A:77:GLN:C	2.72	0.42
1:B:52:ASN:O	1:B:56:LYS:HB2	2.19	0.42
1:B:87:ASP:O	1:B:90:ALA:HB3	2.19	0.42
1:A:170:ASN:CG	1:A:170:ASN:O	2.58	0.42
1:A:370:ILE:HG21	1:A:376:LEU:CD1	2.50	0.42
1:B:146:PHE:CD1	1:B:146:PHE:N	2.87	0.42
1:B:283:SER:O	1:B:284:VAL:CG2	2.58	0.42
1:A:311:ALA:O	1:A:332:GLN:HA	2.20	0.42
1:A:420:ARG:NH2	1:A:441:GLU:OE2	2.53	0.42
1:B:221:TYR:CE2	1:B:300:ARG:HD2	2.54	0.42
1:A:54:LEU:HD13	1:A:54:LEU:HA	1.86	0.42
1:B:178:SER:C	1:B:180:GLU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:SER:HA	1:B:392:TRP:CD1	2.54	0.42
1:B:85:GLN:O	1:B:88:ARG:HB3	2.19	0.42
1:A:101:ASN:HB2	1:A:405:THR:CG2	2.49	0.42
1:A:43:ALA:CB	1:A:159:ARG:HH12	2.33	0.42
1:A:189:ASP:OD2	1:A:189:ASP:C	2.58	0.42
1:A:389:GLU:O	1:A:391:SER:N	2.53	0.42
1:A:485:PHE:C	1:A:485:PHE:CD1	2.93	0.42
1:A:90:ALA:O	1:A:91:MET:C	2.58	0.42
1:B:412:GLU:OE1	1:B:520:GLU:HG2	2.20	0.42
1:A:97:ARG:NH2	1:A:400:LEU:O	2.46	0.41
1:A:49:PHE:CE1	1:A:53:GLU:OE2	2.73	0.41
1:A:504:LEU:HB3	1:A:506:LEU:HD11	2.01	0.41
1:B:105:HIS:O	1:B:311:ALA:HA	2.20	0.41
1:B:312:GLY:C	1:B:313:ILE:HD12	2.40	0.41
1:A:306:THR:O	1:A:306:THR:HG22	2.20	0.41
1:B:438:LEU:O	1:B:439:CYS:C	2.57	0.41
1:B:464:ASN:C	1:B:465:PHE:HD1	2.24	0.41
1:B:294:VAL:O	1:B:298:ARG:HB2	2.20	0.41
1:A:304:LYS:HG2	1:A:304:LYS:O	2.20	0.41
1:A:75:THR:HG23	1:A:78:GLN:CD	2.40	0.41
1:B:427:LYS:HD2	1:B:427:LYS:N	2.34	0.41
1:B:478:VAL:HG12	1:B:479:SER:N	2.35	0.41
1:B:504:LEU:O	1:B:504:LEU:CD1	2.68	0.41
1:A:391:SER:OG	3:T:12:DT:OP1	2.36	0.41
1:A:360:VAL:HG23	2:P:11:DT:OP2	2.20	0.41
1:A:36:ILE:CG2	1:A:160:LEU:HD13	2.50	0.41
1:A:407:LEU:O	1:A:408:THR:C	2.59	0.41
1:A:448:LYS:HE3	1:A:448:LYS:HB2	1.95	0.41
1:B:326:LYS:HZ1	1:B:345:PHE:HE1	1.69	0.41
1:B:433:SER:C	1:B:435:CYS:H	2.24	0.41
2:E:7:DA:C2	2:E:8:DG:C2	3.08	0.41
1:A:105:HIS:CD2	1:A:201:TYR:CE1	3.08	0.41
1:B:42:GLU:OE1	1:B:42:GLU:HA	2.20	0.41
1:B:443:ALA:O	1:B:446:LEU:N	2.53	0.41
2:P:8:DG:H1'	2:P:9:DG:H5''	2.03	0.41
1:A:128:ILE:CD1	1:A:128:ILE:C	2.89	0.41
1:A:282:ASN:ND2	1:A:283:SER:H	2.19	0.41
1:A:516:PHE:N	1:A:516:PHE:CD1	2.89	0.41
1:B:195:MET:HB2	1:B:199:GLU:HG3	2.03	0.41
1:B:417:SER:HB3	1:B:512:ARG:HB2	2.01	0.41
1:A:77:GLN:O	1:A:80:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DA:H2''	2:P:7:DA:H5'	2.02	0.41
1:A:104:VAL:HG12	1:A:105:HIS:N	2.36	0.41
1:A:189:ASP:HA	1:A:190:PRO:HD2	1.83	0.41
1:A:382:LEU:HD23	1:A:386:LEU:HG	2.03	0.41
1:A:451:LEU:HB3	1:A:516:PHE:CD2	2.55	0.41
1:A:47:SER:OG	1:A:49:PHE:HB3	2.21	0.41
1:A:71:LYS:C	1:A:73:GLN:N	2.74	0.41
1:A:135:MET:SD	1:A:151:ALA:HA	2.60	0.40
1:A:186:ALA:C	1:A:188:TYR:N	2.75	0.40
1:A:440:SER:O	1:A:444:GLN:HB2	2.21	0.40
1:A:467:VAL:CG1	1:A:468:LYS:H	2.33	0.40
1:B:328:LYS:HG3	1:B:328:LYS:O	2.21	0.40
1:B:63:ARG:CZ	1:B:364:MET:CE	2.99	0.40
1:B:82:ALA:HB2	1:B:385:LEU:HD21	2.03	0.40
1:B:45:LYS:HG3	1:B:46:GLY:N	2.35	0.40
1:A:432:TYR:O	1:A:435:CYS:HB3	2.21	0.40
1:B:45:LYS:CG	1:B:46:GLY:N	2.84	0.40
3:F:4:DC:C6	3:F:4:DC:H5'	2.54	0.40
1:A:222:PHE:N	1:A:222:PHE:CD1	2.77	0.40
1:A:304:LYS:O	1:A:305:THR:HG23	2.21	0.40
1:A:385:LEU:C	1:A:386:LEU:HD23	2.40	0.40
1:B:120:ASN:HD22	1:B:120:ASN:C	2.24	0.40
1:B:305:THR:O	1:B:306:THR:HB	2.20	0.40
1:A:170:ASN:ND2	1:A:170:ASN:O	2.55	0.40
1:A:370:ILE:HG21	1:A:376:LEU:HD13	2.02	0.40
1:A:420:ARG:C	1:A:508:LEU:HD23	2.42	0.40
1:A:470:ARG:HG3	1:A:495:GLU:OE2	2.21	0.40
1:A:85:GLN:O	1:A:88:ARG:HB3	2.20	0.40
1:A:451:LEU:HB3	1:A:516:PHE:HD2	1.86	0.40
1:B:484:ILE:C	1:B:486:ALA:N	2.73	0.40
3:T:13:DT:H2''	3:T:14:DC:H5'	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/508 (84%)	312 (73%)	86 (20%)	30 (7%)	1	16
1	B	427/508 (84%)	290 (68%)	87 (20%)	50 (12%)	0	5
All	All	855/1016 (84%)	602 (70%)	173 (20%)	80 (9%)	0	9

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	124	LYS
1	A	193	MET
1	A	478	VAL
1	A	501	PRO
1	B	40	ILE
1	B	120	ASN
1	B	121	PRO
1	B	129	ALA
1	B	171	PHE
1	B	186	ALA
1	B	220	ARG
1	B	330	ASN
1	B	410	ASP
1	B	413	ARG
1	B	424	GLU
1	B	449	GLU
1	B	450	ARG
1	B	477	VAL
1	B	481	ALA
1	B	486	ALA
1	B	498	ALA
1	A	72	ALA
1	A	122	GLU
1	A	183	GLU
1	A	187	ASP
1	A	223	ILE
1	A	388	SER
1	A	476	SER
1	B	41	MET
1	B	73	GLN
1	B	122	GLU
1	B	127	PRO

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Mol	Chain	Res	Type
1	B	150	ALA
1	B	170	ASN
1	B	183	GLU
1	B	185	LEU
1	B	204	ILE
1	B	212	GLN
1	B	221	TYR
1	B	283	SER
1	B	340	GLN
1	B	388	SER
1	B	411	GLY
1	B	462	ASN
1	A	45	LYS
1	A	204	ILE
1	A	304	LYS
1	A	355	SER
1	A	390	THR
1	A	438	LEU
1	B	111	PHE
1	B	124	LYS
1	B	190	PRO
1	B	284	VAL
1	B	339	ARG
1	B	381	ALA
1	A	356	GLY
1	A	408	THR
1	A	428	ALA
1	A	439	CYS
1	A	519	GLU
1	B	45	LYS
1	B	72	ALA
1	B	304	LYS
1	B	305	THR
1	B	306	THR
1	B	478	VAL
1	A	305	THR
1	A	340	GLN
1	B	88	ARG
1	B	128	ILE
1	B	184	ILE
1	B	362	GLU
1	A	86	VAL

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Mol	Chain	Res	Type
1	A	129	ALA
1	A	411	GLY
1	A	413	ARG
1	B	173	LYS
1	A	127	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/454 (85%)	334 (87%)	50 (13%)	4	23
1	B	383/454 (84%)	324 (85%)	59 (15%)	2	17
All	All	767/908 (84%)	658 (86%)	109 (14%)	3	20

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	75	THR
1	A	77	GLN
1	A	80	ARG
1	A	83	GLN
1	A	85	GLN
1	A	99	LEU
1	A	100	SER
1	A	118	ARG
1	A	120	ASN
1	A	135	MET
1	A	140	ASN
1	A	149	ARG
1	A	191	ASN
1	A	195	MET
1	A	205	THR
1	A	214	TRP
1	A	220	ARG

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Mol	Chain	Res	Type
1	A	222	PHE
1	A	282	ASN
1	A	288	THR
1	A	318	MET
1	A	325	ASP
1	A	374	THR
1	A	379	GLN
1	A	385	LEU
1	A	395	PHE
1	A	396	LEU
1	A	404	SER
1	A	405	THR
1	A	409	ARG
1	A	410	ASP
1	A	412	GLU
1	A	413	ARG
1	A	416	MET
1	A	421	THR
1	A	422	PHE
1	A	429	GLU
1	A	431	GLN
1	A	444	GLN
1	A	455	THR
1	A	458	ILE
1	A	477	VAL
1	A	480	THR
1	A	482	GLU
1	A	493	LYS
1	A	497	ASP
1	A	499	ASP
1	A	501	PRO
1	A	508	LEU
1	B	33	LYS
1	B	35	LYS
1	B	42	GLU
1	B	50	TYR
1	B	52	ASN
1	B	70	GLN
1	B	73	GLN
1	B	75	THR
1	B	77	GLN
1	B	78	GLN

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	109	ASP
1	B	120	ASN
1	B	121	PRO
1	B	124	LYS
1	B	127	PRO
1	B	128	ILE
1	B	135	MET
1	B	136	LEU
1	B	140	ASN
1	B	155	PHE
1	B	160	LEU
1	B	171	PHE
1	B	172	ASP
1	B	187	ASP
1	B	192	PHE
1	B	212	GLN
1	B	217	ASP
1	B	222	PHE
1	B	325	ASP
1	B	336	LEU
1	B	339	ARG
1	B	340	GLN
1	B	352	ARG
1	B	363	LYS
1	B	372	THR
1	B	374	THR
1	B	379	GLN
1	B	382	LEU
1	B	393	HIS
1	B	397	HIS
1	B	421	THR
1	B	427	LYS
1	B	434	LEU
1	B	441	GLU
1	B	451	LEU
1	B	454	ARG
1	B	457	THR
1	B	466	GLU
1	B	469	THR
1	B	473	THR
1	B	480	THR

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Mol	Chain	Res	Type
1	B	482	GLU
1	B	483	GLU
1	B	504	LEU
1	B	505	ARG
1	B	511	VAL
1	B	518	ASN
1	B	520	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	ASN
1	A	69	GLN
1	A	73	GLN
1	A	77	GLN
1	A	83	GLN
1	A	95	GLN
1	A	101	ASN
1	A	120	ASN
1	A	140	ASN
1	A	163	GLN
1	A	170	ASN
1	A	213	ASN
1	A	282	ASN
1	A	291	GLN
1	A	330	ASN
1	A	340	GLN
1	A	378	GLN
1	A	379	GLN
1	A	397	HIS
1	A	431	GLN
1	A	436	GLN
1	A	462	ASN
1	B	73	GLN
1	B	83	GLN
1	B	95	GLN
1	B	101	ASN
1	B	120	ASN
1	B	203	ASN
1	B	316	ASN
1	B	327	ASN

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Mol	Chain	Res	Type
1	B	330	ASN
1	B	334	GLN
1	B	338	ASN
1	B	379	GLN
1	B	447	GLN
1	B	502	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$
3	8OG	F	5	3	18,25,26	1.34	2 (11%)	21,37,40	2.27	5 (23%)
3	8OG	T	5	3	18,25,26	1.29	2 (11%)	21,37,40	2.32	6 (28%)

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
3	8OG	F	5	3	-	0/3/21/22	0/3/3/3
3	8OG	T	5	3	-	0/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	8OG	C6-N1	4.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	8OG	C6-N1	4.16	1.40	1.33
3	F	5	8OG	C2-N1	2.97	1.40	1.35
3	T	5	8OG	C2-N1	2.87	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	C2-N3-C4	6.01	122.23	115.36
3	T	5	8OG	N3-C2-N1	-5.74	119.56	127.22
3	F	5	8OG	C2-N3-C4	5.73	121.90	115.36
3	F	5	8OG	N3-C2-N1	-5.60	119.76	127.22
3	T	5	8OG	C2'-C1'-N9	-3.56	112.12	116.01
3	F	5	8OG	C5-C6-N1	-3.10	119.20	123.43
3	F	5	8OG	C2'-C1'-N9	-3.00	112.73	116.01
3	T	5	8OG	C5-C6-N1	-2.76	119.66	123.43
3	T	5	8OG	C6-C5-C4	-2.24	118.66	120.80
3	F	5	8OG	C6-N1-C2	2.13	119.32	115.93
3	T	5	8OG	C6-N1-C2	2.03	119.15	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	8OG	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
4	DTP	B	1521	5	26,32,32	0.83	1 (3%)	30,50,50	0.94	3 (10%)
4	DTP	A	1521	5	26,32,32	1.01	2 (7%)	30,50,50	1.02	3 (10%)

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
4	DTP	B	1521	5	-	3/18/34/34	0/3/3/3
4	DTP	A	1521	5	-	3/18/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1521	DTP	C8-N7	-2.38	1.30	1.34
4	A	1521	DTP	C2-N3	2.24	1.35	1.32
4	B	1521	DTP	C2-N3	2.05	1.35	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1521	DTP	PB-O3B-PG	-2.44	124.44	132.83
4	A	1521	DTP	PA-O3A-PB	-2.44	124.47	132.83
4	B	1521	DTP	PB-O3B-PG	-2.39	124.64	132.83
4	B	1521	DTP	O2G-PG-O3B	2.24	112.16	104.64
4	B	1521	DTP	PA-O3A-PB	-2.21	125.26	132.83
4	A	1521	DTP	C4-C5-N7	2.15	111.64	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1521	DTP	C4'-C5'-O5'-PA
4	B	1521	DTP	C3'-C4'-C5'-O5'
4	B	1521	DTP	PG-O3B-PB-O2B
4	A	1521	DTP	PB-O3A-PA-O1A

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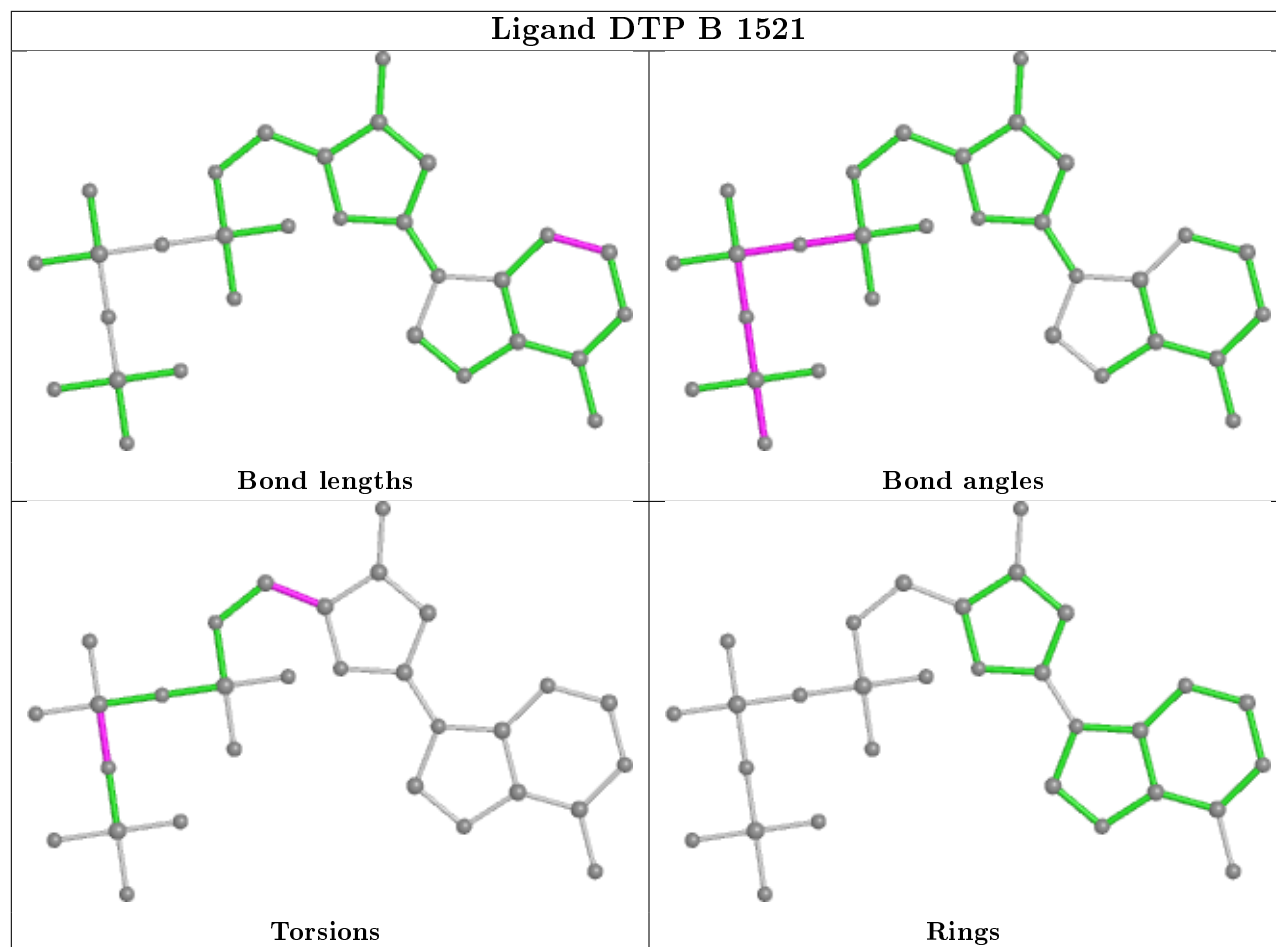
Mol	Chain	Res	Type	Atoms
4	A	1521	DTP	PG-O3B-PB-O1B
4	B	1521	DTP	PG-O3B-PB-O1B

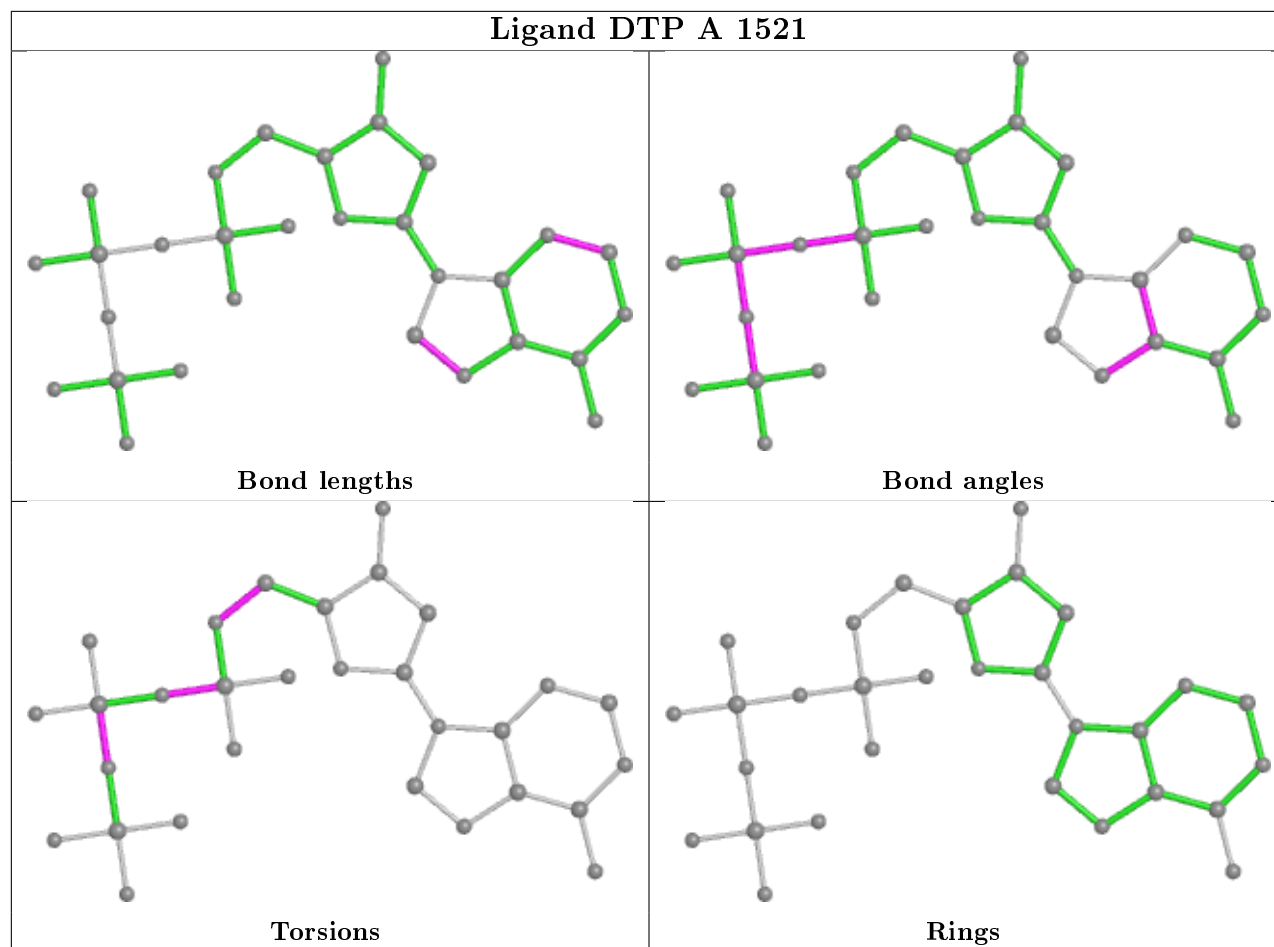
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1521	DTP	1	0
4	A	1521	DTP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/508 (85%)	-0.40	2 (0%) 91 89	49, 77, 117, 128	36 (8%)
1	B	431/508 (84%)	-0.17	2 (0%) 91 89	57, 106, 138, 154	62 (14%)
2	E	11/13 (84%)	-0.55	0 100 100	90, 114, 153, 153	2 (18%)
2	P	13/13 (100%)	-0.24	0 100 100	65, 103, 171, 171	0
3	F	14/18 (77%)	-0.10	0 100 100	98, 115, 169, 176	1 (7%)
3	T	16/18 (88%)	-0.28	0 100 100	80, 97, 153, 155	0
All	All	917/1078 (85%)	-0.28	4 (0%) 92 91	49, 91, 134, 176	101 (11%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	ASN	2.8
1	B	409	ARG	2.6
1	A	518	ASN	2.2
1	A	517	PRO	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8OG	F	5	23/24	0.92	0.19	104,110,114,117	0
3	8OG	T	5	23/24	0.96	0.17	77,81,84,90	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

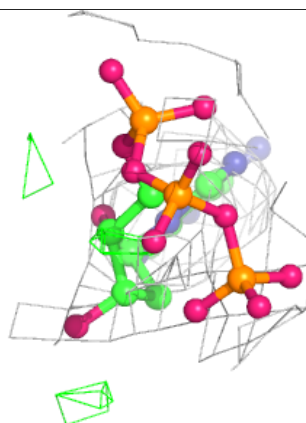
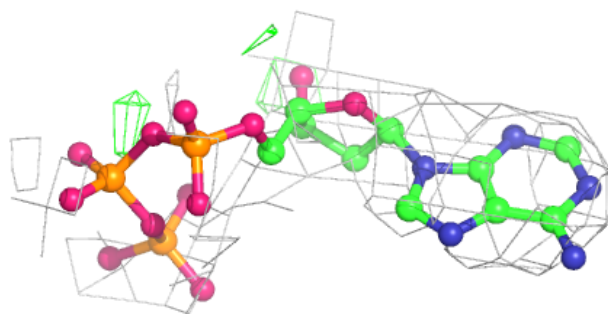
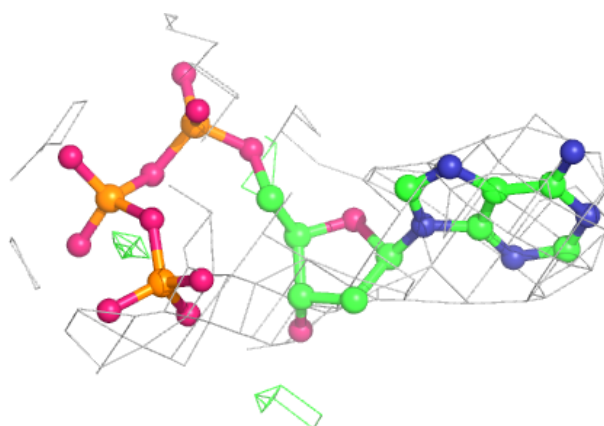
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DTP	B	1521	30/30	0.91	0.26	135,144,156,157	0
5	CA	B	1522	1/1	0.91	0.21	88,88,88,88	0
5	CA	A	1522	1/1	0.95	0.15	64,64,64,64	0
4	DTP	A	1521	30/30	0.96	0.19	91,100,109,110	0
5	CA	B	1523	1/1	0.98	0.24	94,94,94,94	0
5	CA	A	1523	1/1	0.99	0.17	67,67,67,67	0

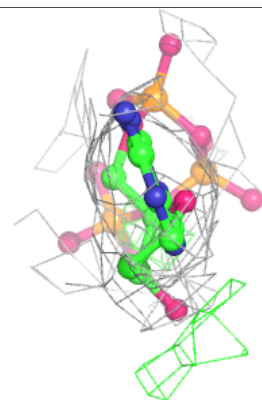
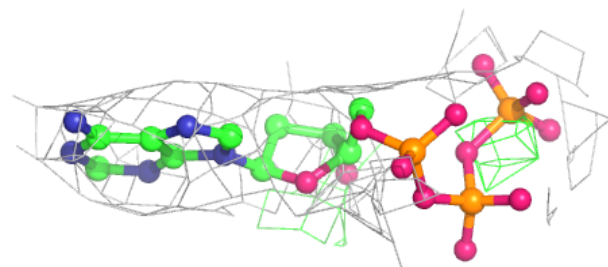
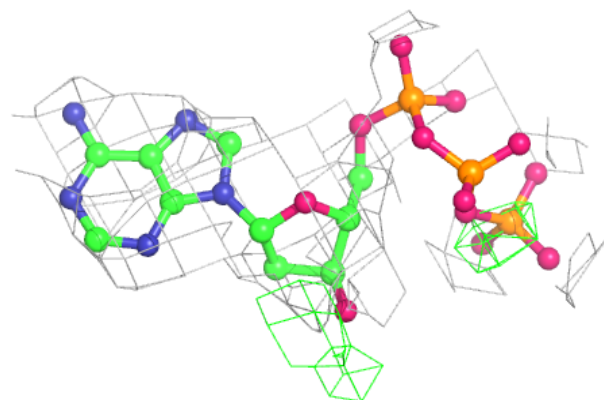
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP B 1521:

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

**Electron density around DTP A 1521:**

$2mF_o-DF_c$ (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.