



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:33 pm BST

PDB ID : 4TQS
Title : Ternary complex of Y-family DNA polymerase Dpo4 with (5'S)-8,5'-Cyclo-2'-deoxyguanosine and dCTP
Authors : Zhao, L.
Deposited on : 2014-06-11
Resolution : 2.06 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

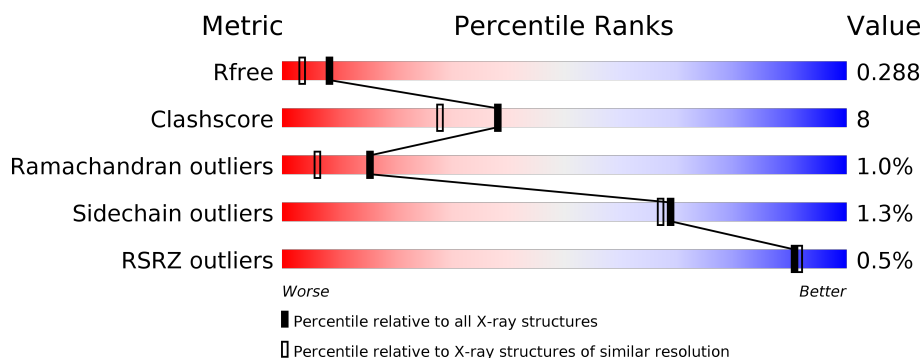
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	358	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	358	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	C	12	<div> <div></div> <div>100%</div> </div>
2	P	12	<div> <div></div> <div>67%</div> <div>33%</div> </div>
3	D	18	<div> <div></div> <div>39%</div> <div>33%</div> <div>28%</div> </div>
3	T	18	<div> <div></div> <div>56%</div> <div>22%</div> <div>22%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6849 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2573	1655	427	485	6			
1	B	343	Total	C	N	O	S	0	0	0
			2648	1706	446	489	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q97W02
A	-4	HIS	-	expression tag	UNP Q97W02
A	-3	HIS	-	expression tag	UNP Q97W02
A	-2	HIS	-	expression tag	UNP Q97W02
A	-1	HIS	-	expression tag	UNP Q97W02
A	0	HIS	-	expression tag	UNP Q97W02
B	-5	HIS	-	expression tag	UNP Q97W02
B	-4	HIS	-	expression tag	UNP Q97W02
B	-3	HIS	-	expression tag	UNP Q97W02
B	-2	HIS	-	expression tag	UNP Q97W02
B	-1	HIS	-	expression tag	UNP Q97W02
B	0	HIS	-	expression tag	UNP Q97W02

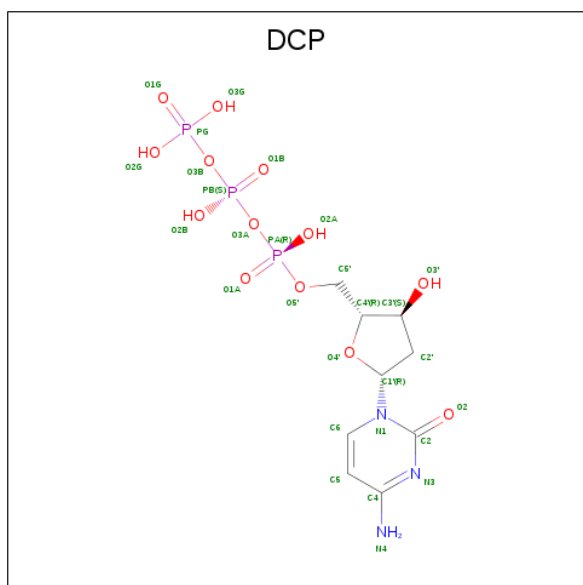
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			254	120	54	69	11			
2	P	12	Total	C	N	O	P	0	0	0
			254	120	54	69	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			257	123	42	79	13			
3	T	14	Total	C	N	O	P	0	0	0
			279	133	47	85	14			

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).

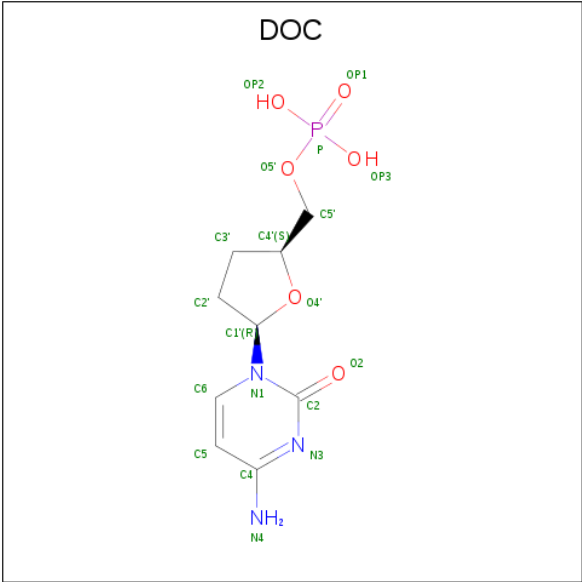


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
4	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

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

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

- Molecule 6 is 2',3'-DIDEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DOC) (formula: $C_9H_{14}N_3O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
6	P	1	Total	C	N	O	P	0	0
			18	9	3	5	1		

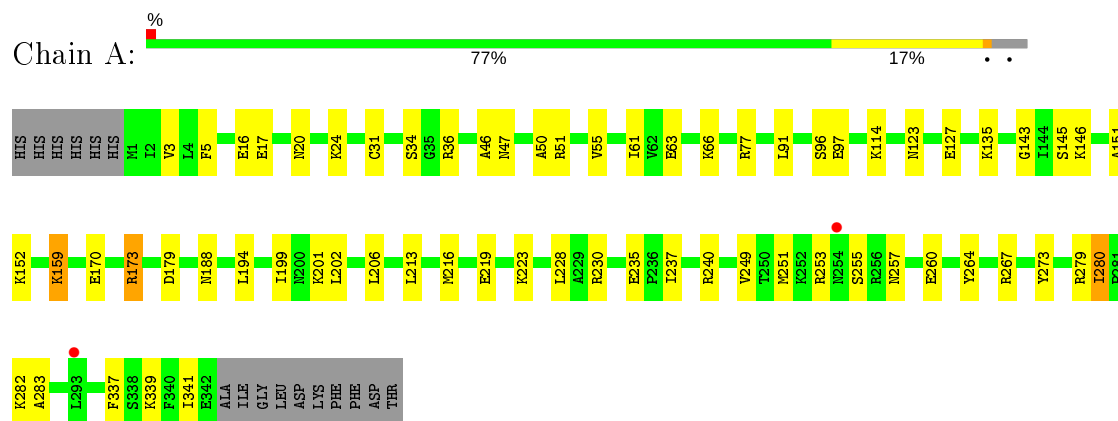
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		
7	B	202	Total	O	0	0
			202	202		
7	C	28	Total	O	0	0
			28	28		
7	D	24	Total	O	0	0
			24	24		
7	P	20	Total	O	0	0
			20	20		
7	T	37	Total	O	0	0
			37	37		

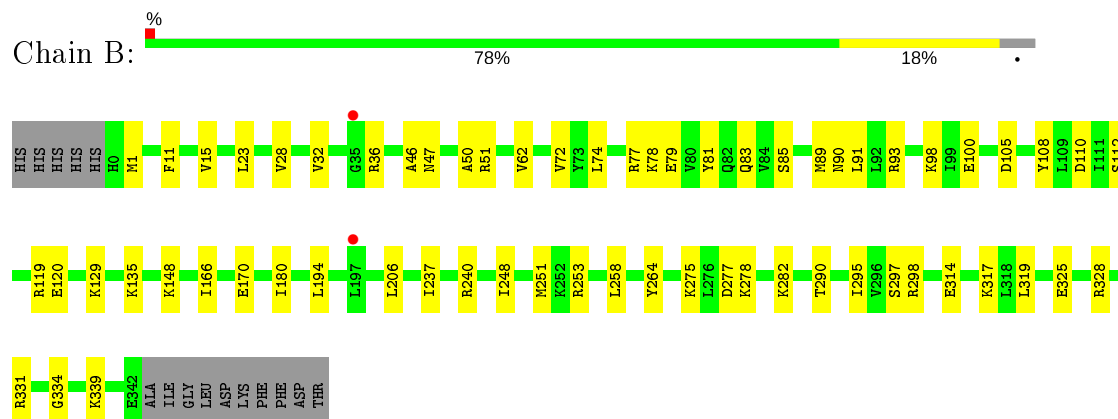
3 Residue-property plots

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 polymerase IV



- Molecule 1: DNA polymerase IV



- Molecule 2: DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*T)-3')



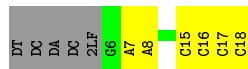
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*T)-3')

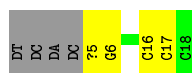




- Molecule 3: DNA (5'-D(P*TP*CP*AP*CP*(2LF)P*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.12Å 184.24Å 52.12Å 90.00° 110.09° 90.00°	Depositor
Resolution (Å)	28.41 – 2.06 28.41 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.41-2.06) 97.6 (28.41-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.228 , 0.290 0.229 , 0.288	Depositor DCC
R_{free} test set	2859 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.388 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6849	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, 2LF, DCP

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	0.51	0/2610	0.59	1/3536 (0.0%)
1	B	0.46	0/2687	0.55	0/3626
2	C	0.89	0/287	0.84	0/444
2	P	0.90	2/287 (0.7%)	0.93	0/444
3	D	0.78	0/285	0.96	0/435
3	T	0.86	0/285	0.90	0/435
All	All	0.57	2/6441 (0.0%)	0.65	1/8920 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	12	DT	P-OP2	-5.62	1.39	1.49
2	P	12	DT	P-OP1	-5.19	1.40	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LYS	C-N-CD	5.29	139.52	128.40

There are no chirality outliers.

There are no planarity outliers.

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	2573	0	2544	40	0
1	B	2648	0	2704	40	0
2	C	254	0	135	0	0
2	P	254	0	135	4	0
3	D	257	0	147	7	0
3	T	279	0	156	2	0
4	A	28	0	12	1	0
4	B	28	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	C	18	0	12	0	0
6	P	18	0	12	0	0
7	A	177	0	0	5	1
7	B	202	0	0	3	0
7	C	28	0	0	0	1
7	D	24	0	0	0	0
7	P	20	0	0	0	0
7	T	37	0	0	0	0
All	All	6849	0	5869	92	1

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 8.

All (92) 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:170:GLU:OE1	1:A:173:ARG:NH1	1.88	1.06
1:B:298:ARG:NH2	1:B:325:GLU:OE1	2.15	0.78
1:A:179:ASP:OD1	1:A:201:LYS:NZ	2.23	0.71
1:A:63:GLU:HA	1:A:66:LYS:HE2	1.73	0.69
1:A:279:ARG:O	1:A:280:ILE:HB	1.91	0.69
1:B:32:VAL:HG11	3:D:7:DA:H5'	1.74	0.68
1:B:91:LEU:HD21	1:B:135:LYS:HE2	1.76	0.65
1:B:248:ILE:HG13	1:B:334:GLY:HA3	1.77	0.65
1:A:283:ALA:HB2	1:A:339:LYS:HD2	1.83	0.61
1:B:108:TYR:CD1	1:B:148:LYS:HG2	2.36	0.61
2:P:3:DG:H5''	2:P:3:DG:H8	1.65	0.60
1:A:280:ILE:HG21	1:A:341:ILE:HG13	1.83	0.59
1:B:248:ILE:HA	1:B:334:GLY:HA3	1.85	0.57
1:A:280:ILE:HG22	1:A:341:ILE:HG12	1.86	0.57
1:B:110:ASP:HB2	1:B:237:ILE:HG12	1.87	0.56
1:B:314:GLU:HA	1:B:317:LYS:NZ	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HA	1:B:317:LYS:HZ3	1.71	0.56
1:B:90:ASN:HA	1:B:93:ARG:HG3	1.88	0.55
1:B:23:LEU:HD22	1:B:72:VAL:HG11	1.89	0.55
1:A:249:VAL:HG21	1:A:267:ARG:HH21	1.70	0.55
1:A:280:ILE:CG2	1:A:341:ILE:CG1	2.85	0.54
1:A:257:ASN:HB3	1:A:260:GLU:HB2	1.90	0.53
1:B:166:ILE:HG23	1:B:170:GLU:CG	2.38	0.53
3:D:16:DC:H2'	3:D:17:DC:C6	2.43	0.53
1:A:3:VAL:HG13	1:A:237:ILE:HD11	1.91	0.53
1:B:98:LYS:HB2	1:B:110:ASP:HB3	1.90	0.52
1:A:16:GLU:OE2	1:A:77:ARG:HD3	2.09	0.52
1:A:170:GLU:CD	1:A:173:ARG:HH12	2.12	0.52
1:A:77:ARG:HD2	7:A:664:HOH:O	2.10	0.51
1:A:50:ALA:O	1:A:55:VAL:HG22	2.10	0.51
1:A:280:ILE:CG2	1:A:341:ILE:HG13	2.41	0.51
1:B:77:ARG:HD2	7:B:537:HOH:O	2.10	0.51
1:A:20:ASN:HB2	7:A:633:HOH:O	2.10	0.50
1:A:188:ASN:ND2	7:A:612:HOH:O	2.41	0.49
1:B:282:LYS:HE2	1:B:339:LYS:O	2.12	0.49
1:A:123:ASN:O	1:A:127:GLU:HG3	2.12	0.49
1:A:251:MET:HA	1:A:264:TYR:CE1	2.48	0.48
1:A:280:ILE:CG2	1:A:341:ILE:HG12	2.43	0.48
1:B:46:ALA:HB1	1:B:50:ALA:HB3	1.96	0.48
1:B:15:VAL:HG11	1:B:81:TYR:CD1	2.48	0.48
1:A:31:CYS:HB3	1:A:61:ILE:HD11	1.95	0.47
4:A:401:DCP:O3'	7:A:602:HOH:O	2.20	0.47
1:B:91:LEU:HD11	1:B:135:LYS:HE3	1.95	0.47
1:A:50:ALA:HB1	1:A:55:VAL:CG2	2.45	0.47
1:B:251:MET:HG2	1:B:331:ARG:O	2.15	0.47
1:A:96:SER:HA	1:A:114:LYS:HE2	1.97	0.47
1:A:282:LYS:HB2	1:A:339:LYS:O	2.16	0.46
1:A:91:LEU:HD21	1:A:135:LYS:HE2	1.96	0.46
1:A:202:LEU:HD21	1:A:228:LEU:HB3	1.98	0.46
1:A:5:PHE:CD2	1:A:152:LYS:HA	2.50	0.46
1:A:97:GLU:H	1:A:97:GLU:CD	2.18	0.46
3:T:5:2LF:H'2'	3:T:6:DG:C5'	2.46	0.46
1:B:98:LYS:C	1:B:237:ILE:HD11	2.36	0.46
1:B:119:ARG:HG3	1:B:120:GLU:N	2.31	0.45
1:B:277:ASP:HB3	1:B:278:LYS:H	1.63	0.45
3:D:17:DC:H4'	3:D:18:DC:OP1	2.17	0.45
1:B:78:LYS:NZ	3:D:8:DA:H4'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:DG:C8	2:P:3:DG:H5"	2.49	0.45
1:A:206:LEU:HD21	1:A:230:ARG:HG3	1.98	0.44
1:A:135:LYS:HE3	1:A:135:LYS:HB3	1.87	0.44
3:D:17:DC:H2'	3:D:18:DC:C6	2.53	0.44
1:B:258:LEU:HD12	1:B:319:LEU:HD23	2.00	0.44
1:B:36:ARG:NH2	7:B:519:HOH:O	2.50	0.44
3:D:17:DC:H2'	3:D:18:DC:C5	2.53	0.43
1:B:248:ILE:HG13	1:B:334:GLY:CA	2.47	0.43
1:B:251:MET:HA	1:B:264:TYR:CE1	2.53	0.43
1:B:85:SER:O	1:B:89:MET:HG2	2.18	0.43
7:A:723:HOH:O	2:P:7:DA:H8	2.01	0.43
3:T:16:DC:H2"	3:T:17:DC:C6	2.54	0.43
1:A:213:LEU:HA	1:A:216:MET:HE2	2.01	0.43
1:A:219:GLU:O	1:A:223:LYS:HG3	2.18	0.42
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.99	0.42
1:B:275:LYS:HD3	1:B:275:LYS:HA	1.66	0.42
3:D:15:DC:H2"	3:D:16:DC:C6	2.55	0.42
1:A:194:LEU:HB3	1:A:199:ILE:HB	2.01	0.42
1:B:129:LYS:HB3	1:B:129:LYS:HE2	1.91	0.42
1:A:17:GLU:HG2	1:A:24:LYS:HA	2.02	0.41
1:B:47:ASN:O	1:B:51:ARG:HG3	2.20	0.41
1:B:166:ILE:HG23	1:B:170:GLU:HG3	2.02	0.41
1:A:273:TYR:HE2	1:A:337:PHE:CZ	2.39	0.41
1:B:100:GLU:HG3	1:B:240:ARG:HG2	2.03	0.41
1:B:28:VAL:HG13	1:B:74:LEU:HD13	2.02	0.41
1:A:145:SER:OG	1:A:146:LYS:N	2.52	0.41
1:A:47:ASN:O	1:A:51:ARG:HG3	2.21	0.41
1:B:290:THR:HG21	1:B:328:ARG:HE	1.85	0.41
1:B:62:VAL:HG23	7:B:594:HOH:O	2.20	0.41
1:B:79:GLU:O	1:B:83:GLN:HG3	2.21	0.41
1:B:180:ILE:HG21	1:B:194:LEU:HD12	2.03	0.41
1:A:143:GLY:HA3	1:A:151:ALA:O	2.20	0.40
2:P:3:DG:H2'	2:P:4:DG:C8	2.56	0.40
1:B:1:MET:HA	1:B:112:SER:OG	2.22	0.40
1:B:11:PHE:O	1:B:15:VAL:HG12	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:775:HOH:O	7:C:227:HOH:O[2_546]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/358 (95%)	317 (93%)	17 (5%)	6 (2%)	8	2
1	B	341/358 (95%)	332 (97%)	8 (2%)	1 (0%)	41	32
All	All	681/716 (95%)	649 (95%)	25 (4%)	7 (1%)	15	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	159	LYS
1	A	255	SER
1	A	253	ARG
1	A	235	GLU
1	A	280	ILE
1	B	253	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/315 (82%)	254 (99%)	3 (1%)	71	69
1	B	276/315 (88%)	272 (99%)	4 (1%)	67	64
All	All	533/630 (85%)	526 (99%)	7 (1%)	69	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	173	ARG
1	A	240	ARG
1	B	105	ASP
1	B	206	LEU
1	B	295	ILE
1	B	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	2LF	T	5	3	17,25,26	4.59	10 (58%)	17,39,42	2.43	8 (47%)

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	2LF	T	5	3	-	0/0/28/29	0/3/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	2LF	O4'-C4'	-12.60	1.25	1.44
3	T	5	2LF	C4-N3	6.64	1.46	1.35
3	T	5	2LF	C6-C5	5.41	1.50	1.41
3	T	5	2LF	O4'-C1'	-4.96	1.31	1.42
3	T	5	2LF	C2-N1	4.83	1.44	1.35
3	T	5	2LF	C6-N1	4.77	1.41	1.33
3	T	5	2LF	C2-N2	4.30	1.42	1.33
3	T	5	2LF	O3'-C3'	-3.57	1.35	1.43
3	T	5	2LF	C8-C5'	3.47	1.57	1.51
3	T	5	2LF	C2-N3	2.32	1.45	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	2LF	N3-C2-N1	-5.55	119.82	127.22
3	T	5	2LF	C2-N3-C4	4.40	120.39	115.36
3	T	5	2LF	O4'-C1'-C2'	-2.89	100.78	106.25
3	T	5	2LF	C2'-C1'-N9	-2.66	105.37	109.56
3	T	5	2LF	C6-N1-C2	2.56	120.00	115.93
3	T	5	2LF	C2'-C3'-C4'	-2.28	100.26	103.23
3	T	5	2LF	C5-C6-N1	-2.28	120.31	123.43
3	T	5	2LF	O3'-C3'-C2'	2.04	118.21	110.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	2LF	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	DCP	A	401	5	23,29,29	3.46	11 (47%)	30,45,45	1.52	6 (20%)
6	DOC	C	101	2,5	14,19,20	4.86	11 (78%)	13,26,29	2.97	10 (76%)
4	DCP	B	401	5	23,29,29	3.39	10 (43%)	30,45,45	1.69	6 (20%)
6	DOC	P	101	2,5	14,19,20	4.86	8 (57%)	13,26,29	1.95	3 (23%)

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	DCP	A	401	5	-	2/19/34/34	0/2/2/2
6	DOC	C	101	2,5	-	1/4/18/19	0/2/2/2
4	DCP	B	401	5	-	1/19/34/34	0/2/2/2
6	DOC	P	101	2,5	-	1/4/18/19	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	101	DOC	O4'-C4'	-9.95	1.24	1.44
6	C	101	DOC	O4'-C4'	-9.77	1.25	1.44
4	A	401	DCP	C2'-C3'	-9.40	1.28	1.52
6	C	101	DOC	C2'-C1'	-9.07	1.31	1.51
4	B	401	DCP	C2'-C3'	-9.00	1.29	1.52
6	P	101	DOC	O4'-C1'	8.90	1.62	1.42
6	C	101	DOC	O4'-C1'	8.87	1.62	1.42
6	P	101	DOC	C2'-C1'	-8.12	1.33	1.51
4	B	401	DCP	O4'-C1'	-6.39	1.28	1.42
4	A	401	DCP	O4'-C1'	-6.37	1.28	1.42
4	A	401	DCP	C6-N1	5.71	1.42	1.35
4	B	401	DCP	C6-N1	5.62	1.42	1.35
4	A	401	DCP	C2-N3	4.80	1.47	1.38
6	P	101	DOC	C1'-N1	-4.65	1.35	1.49
4	B	401	DCP	C2-N3	4.62	1.47	1.38
4	A	401	DCP	O3'-C3'	4.42	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	DCP	O3'-C3'	4.33	1.52	1.43
6	P	101	DOC	C6-N1	4.26	1.41	1.35
6	P	101	DOC	C6-C5	4.26	1.47	1.38
4	A	401	DCP	C6-C5	4.21	1.47	1.38
4	B	401	DCP	O4'-C4'	3.86	1.53	1.45
4	B	401	DCP	C4-N3	3.71	1.41	1.35
6	C	101	DOC	C5-C4	3.66	1.50	1.41
6	C	101	DOC	C6-C5	3.63	1.46	1.38
6	C	101	DOC	C2-N3	3.60	1.45	1.38
4	B	401	DCP	C2'-C1'	3.58	1.62	1.52
4	A	401	DCP	O4'-C4'	3.55	1.52	1.45
4	B	401	DCP	C6-C5	3.54	1.45	1.38
6	C	101	DOC	C6-N1	3.50	1.40	1.35
4	A	401	DCP	C4-N3	3.30	1.40	1.35
6	P	101	DOC	O5'-C5'	-3.19	1.37	1.44
4	A	401	DCP	C2'-C1'	3.16	1.61	1.52
4	A	401	DCP	C5'-C4'	-2.98	1.42	1.51
4	B	401	DCP	C5'-C4'	-2.76	1.43	1.51
6	P	101	DOC	C5-C4	2.37	1.46	1.41
6	C	101	DOC	C4-N3	2.28	1.39	1.35
6	C	101	DOC	C1'-N1	-2.21	1.42	1.49
6	C	101	DOC	O5'-C5'	-2.19	1.39	1.44
6	C	101	DOC	C5'-C4'	2.15	1.57	1.50
4	A	401	DCP	C5-C4	2.14	1.46	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	DCP	C2-N3-C4	5.13	121.54	116.34
6	P	101	DOC	C2-N3-C4	4.64	121.04	116.34
6	C	101	DOC	C5-C4-N3	-4.64	116.37	121.72
6	C	101	DOC	C6-N1-C2	-4.26	114.44	121.20
4	A	401	DCP	PB-O3B-PG	-4.10	118.75	132.83
6	C	101	DOC	O4'-C4'-C5'	3.92	115.96	109.52
4	A	401	DCP	C2-N3-C4	3.70	120.10	116.34
6	C	101	DOC	C2'-C1'-N1	3.24	118.59	112.48
4	B	401	DCP	C4'-O4'-C1'	-3.13	101.89	109.45
6	C	101	DOC	C3'-C2'-C1'	3.12	106.39	102.78
6	C	101	DOC	O4'-C1'-C2'	-3.06	103.36	106.67
4	B	401	DCP	N4-C4-N3	2.96	121.17	116.49
6	P	101	DOC	O4'-C1'-C2'	2.94	109.86	106.67
6	C	101	DOC	C5-C4-N4	2.93	126.22	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	DOC	O4'-C4'-C3'	-2.75	100.24	104.80
4	A	401	DCP	C4'-O4'-C1'	-2.65	103.05	109.45
4	B	401	DCP	PB-O3B-PG	-2.61	123.86	132.83
6	C	101	DOC	C2'-C3'-C4'	2.38	107.18	102.72
6	C	101	DOC	C2-N3-C4	2.37	118.74	116.34
6	P	101	DOC	C3'-C2'-C1'	2.20	105.32	102.78
4	A	401	DCP	C3'-C2'-C1'	2.18	107.99	102.54
4	A	401	DCP	C2'-C1'-N1	-2.12	109.39	114.27
4	B	401	DCP	O2A-PA-O5'	2.08	117.42	107.75
4	B	401	DCP	O4'-C4'-C5'	2.06	116.14	109.37
4	A	401	DCP	O2G-PG-O3B	2.03	111.45	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

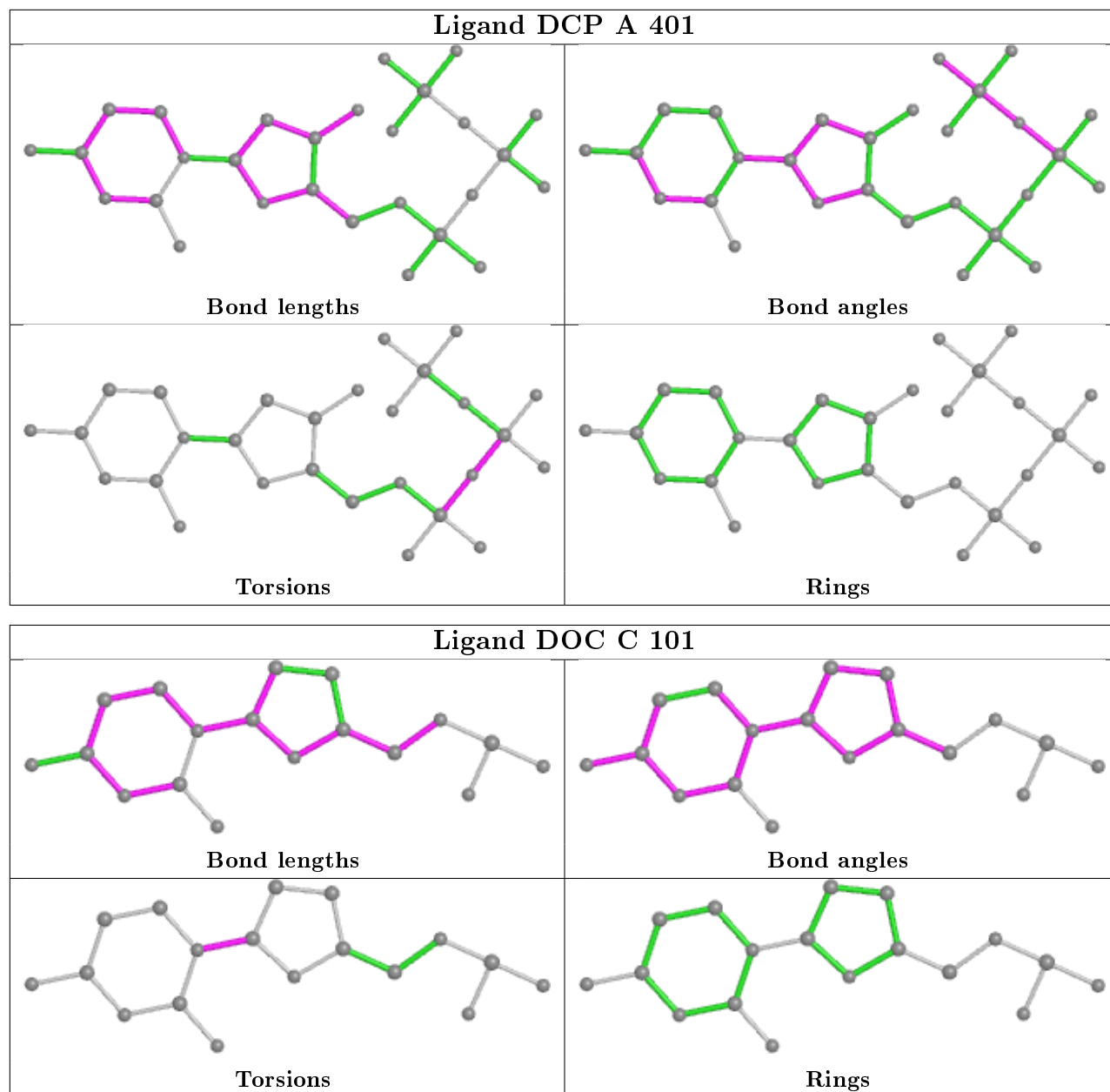
Mol	Chain	Res	Type	Atoms
6	C	101	DOC	O4'-C1'-N1-C6
6	P	101	DOC	O4'-C1'-N1-C6
4	A	401	DCP	PB-O3A-PA-O2A
4	A	401	DCP	PA-O3A-PB-O1B
4	B	401	DCP	PB-O3A-PA-O2A

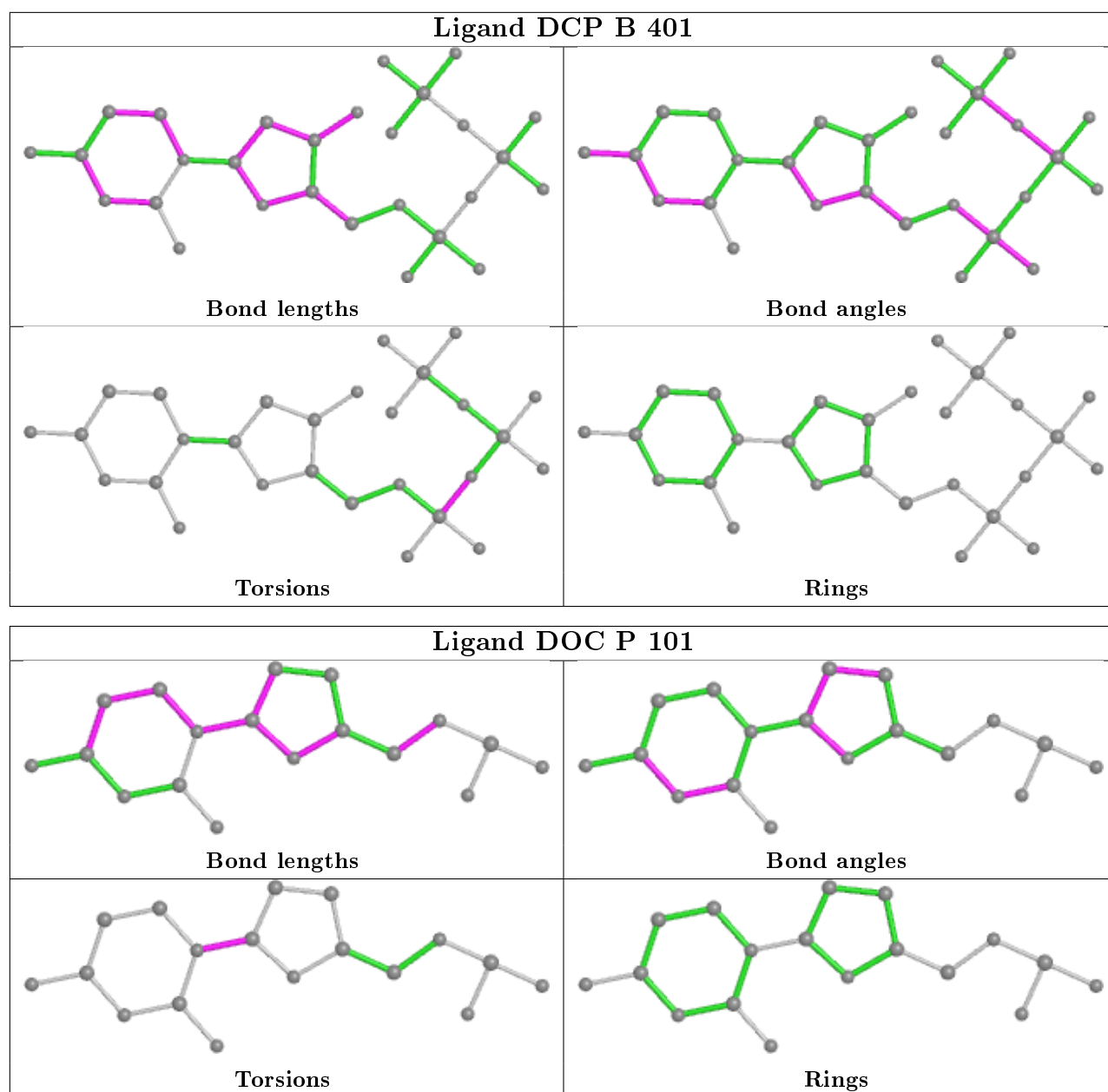
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	DCP	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	342/358 (95%)	-0.25	2 (0%) 89 90	10, 24, 45, 63	0
1	B	343/358 (95%)	-0.27	2 (0%) 89 90	12, 22, 41, 53	0
2	C	12/12 (100%)	-0.61	0 100 100	17, 34, 49, 57	0
2	P	12/12 (100%)	-0.56	0 100 100	14, 28, 47, 48	0
3	D	13/18 (72%)	-0.50	0 100 100	22, 29, 58, 63	0
3	T	13/18 (72%)	-0.46	0 100 100	20, 31, 59, 68	0
All	All	735/776 (94%)	-0.28	4 (0%) 91 91	10, 23, 45, 68	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	ASN	7.1
1	A	293	LEU	5.0
1	B	35	GLY	3.2
1	B	197	LEU	2.5

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	2LF	T	5	22/23	0.70	0.27	61,73,79,80	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

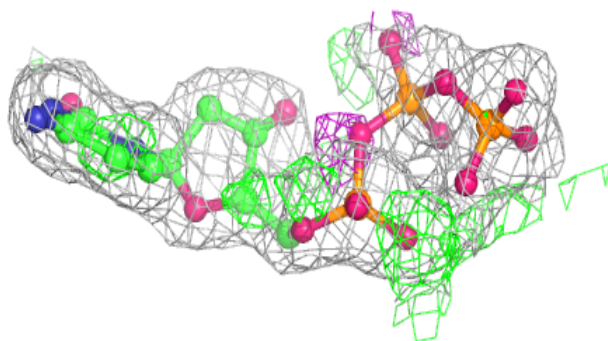
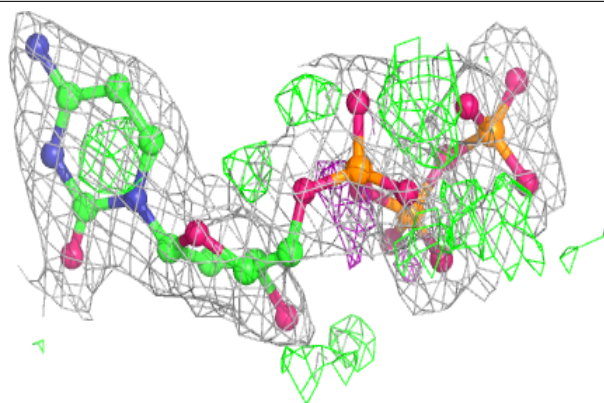
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DCP	B	401	28/28	0.93	0.13	9,20,62,147	0
6	DOC	C	101	18/19	0.94	0.13	15,25,38,40	0
4	DCP	A	401	28/28	0.95	0.10	5,26,38,163	0
6	DOC	P	101	18/19	0.96	0.08	1,22,31,38	0
5	MG	B	403	1/1	0.99	0.16	0,0,0,0	0
5	MG	B	402	1/1	1.00	0.15	0,0,0,0	0
5	MG	A	402	1/1	1.00	0.18	0,0,0,0	0
5	MG	A	403	1/1	1.00	0.12	1,1,1,1	0

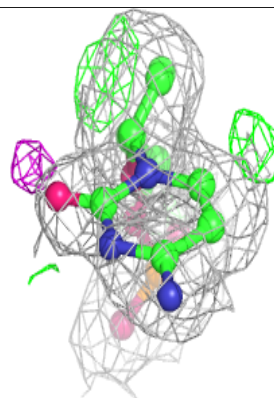
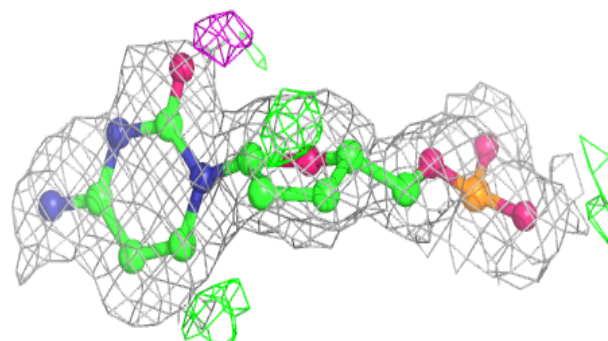
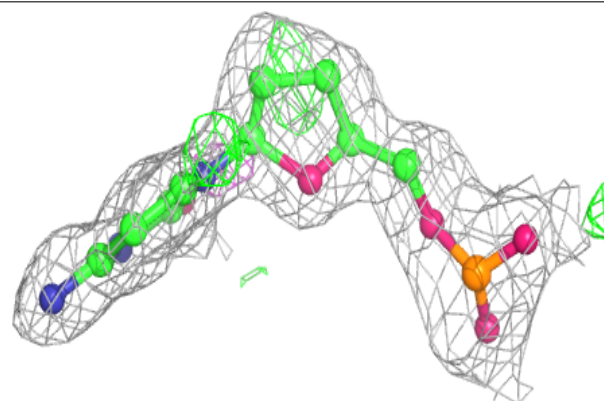
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCP B 401:

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

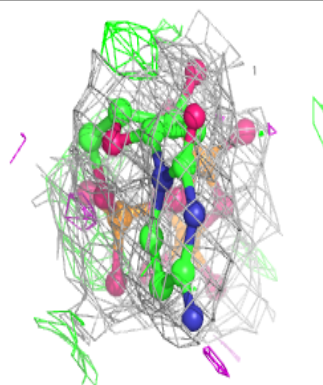
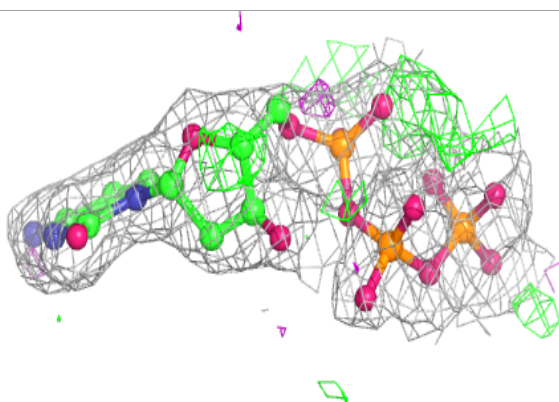
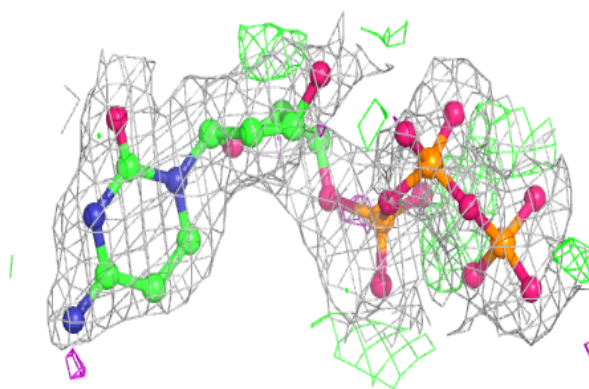
**Electron density around DOC C 101:**

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

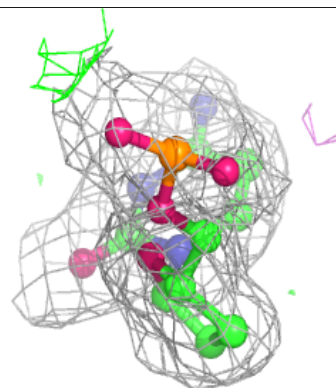
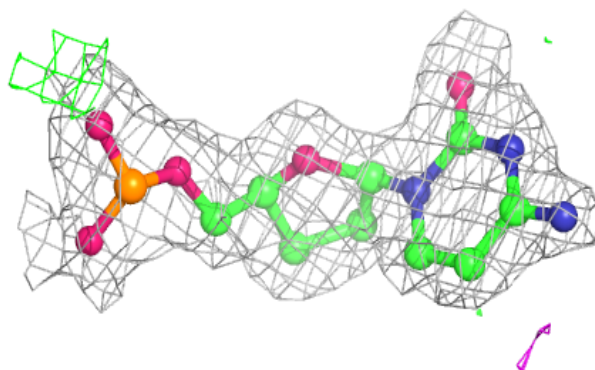
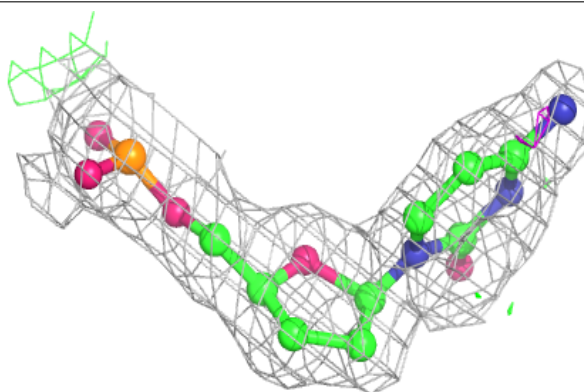


Electron density around DCP A 401:

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

**Electron density around DOC P 101:**

$2mF_o-DF_c$ (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.