



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:25 am BST

PDB ID : 1W2Y  
Title : The crystal structure of a complex of Campylobacter jejuni dUTPase with substrate analogue dUpNHp  
Authors : Moroz, O.V.; Harkiolaki, M.; Galperin, M.Y.; Vagin, A.A.; Gonzalez-Pacanowska, D.; Wilson, K.S.  
Deposited on : 2004-07-09  
Resolution : 1.65 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](mailto: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

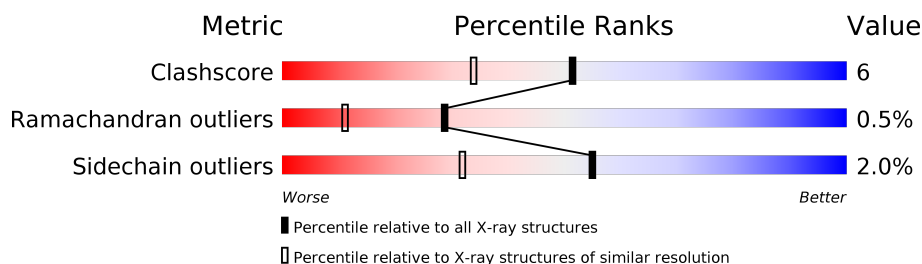
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	229	
1	B	229	

## 2 Entry composition [i](#)

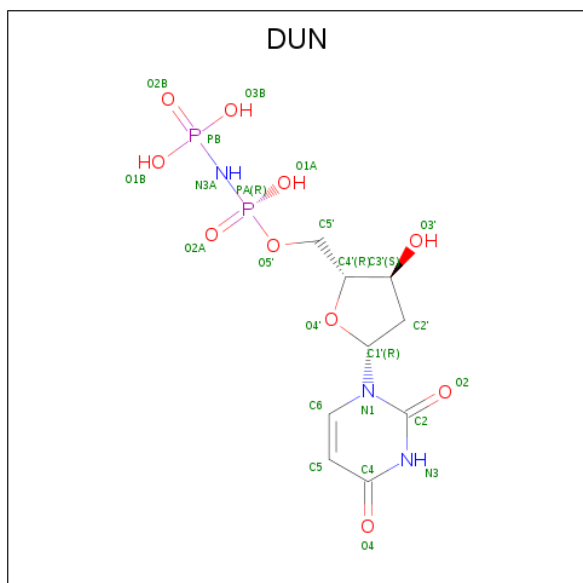
There are 4 unique types of molecules in this entry. The entry contains 4067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	83	4	0
			1895	1220	306	360	9			
1	B	209	Total	C	N	O	S	59	2	0
			1735	1121	285	320	9			

- Molecule 2 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-DIPHOSPHATE (three-letter code: DUN) (formula:  $C_9H_{15}N_3O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	9	3	10	2		
2	B	1	Total	C	N	O	P	0	0
			24	9	3	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total 195	O 195	0	0
4	B	188	Total 188	O 188	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.96Å 70.63Å 92.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.90 – 1.65 48.59 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.90-1.65) 99.0 (48.59-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.151 , 0.194 0.237 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.41	18/1953 (0.9%)	1.56	24/2633 (0.9%)
1	B	1.85	8/1777 (0.5%)	1.14	13/2391 (0.5%)
All	All	1.64	26/3730 (0.7%)	1.38	37/5024 (0.7%)

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	A	2	5
1	B	1	0
All	All	3	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	GLN	CB-CG	-41.82	0.39	1.52
1	B	224	GLU	CB-CG	32.54	2.13	1.52
1	B	146	ASN	CG-OD1	29.28	1.88	1.24
1	B	146	ASN	CG-ND2	-28.83	0.60	1.32
1	A	90	TYR	CB-CG	-20.79	1.20	1.51
1	A	143	PHE	C-N	-17.70	1.01	1.33
1	A	143	PHE	CA-C	-16.14	1.10	1.52
1	A	144	GLY	C-N	-15.52	0.98	1.34
1	A	8	GLU	CB-CG	-14.52	1.24	1.52
1	B	227	LYS	CA-CB	-13.44	1.24	1.53
1	A	94	ASN	CA-CB	-12.12	1.21	1.53
1	B	220	LYS	CA-CB	11.74	1.79	1.53
1	A	227	LYS	CA-CB	-11.23	1.29	1.53
1	B	149	GLU	CA-CB	-11.21	1.29	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLU	CG-CD	10.66	1.68	1.51
1	A	95	ASN	CA-CB	-10.25	1.26	1.53
1	A	145	PHE	N-CA	9.78	1.66	1.46
1	A	197	ASN	CA-CB	-9.55	1.28	1.53
1	A	224	GLU	CG-CD	9.17	1.65	1.51
1	A	112	GLN	CG-CD	8.91	1.71	1.51
1	A	220	LYS	CG-CD	-7.75	1.26	1.52
1	A	166	GLU	CD-OE1	7.25	1.33	1.25
1	A	118	GLU	CD-OE2	6.79	1.33	1.25
1	A	69	GLU	CB-CG	-6.79	1.39	1.52
1	B	221	LYS	CA-CB	6.46	1.68	1.53
1	A	89	GLU	CA-CB	-5.36	1.42	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	O-C-N	-50.35	37.60	123.20
1	A	143	PHE	CA-C-N	23.65	163.50	116.20
1	B	146	ASN	CB-CG-OD1	-19.89	81.83	121.60
1	B	146	ASN	CB-CG-ND2	16.51	156.32	116.70
1	B	221	LYS	N-CA-CB	-16.38	81.12	110.60
1	A	143	PHE	N-CA-C	12.41	144.50	111.00
1	A	143	PHE	C-N-CA	-11.87	97.38	122.30
1	A	224	GLU	CB-CG-CD	-11.80	82.35	114.20
1	B	227	LYS	CB-CA-C	11.34	133.08	110.40
1	B	220	LYS	CB-CA-C	10.05	130.50	110.40
1	B	224	GLU	CA-CB-CG	-8.76	94.14	113.40
1	A	40[A]	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	40[B]	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	119	GLU	CA-CB-CG	8.56	132.23	113.40
1	B	199	LYS	CD-CE-NZ	7.95	129.98	111.70
1	A	90	TYR	CA-CB-CG	7.47	127.59	113.40
1	A	94	ASN	N-CA-CB	7.45	124.01	110.60
1	B	52	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	220	LYS	CB-CG-CD	6.87	129.46	111.60
1	A	120	TYR	CB-CA-C	-6.84	96.72	110.40
1	B	132	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	227	LYS	CB-CA-C	6.66	123.72	110.40
1	A	52	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	227	LYS	N-CA-CB	6.33	121.99	110.60
1	B	201	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	125	ASP	CB-CG-OD2	6.27	123.95	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LYS	N-CA-CB	-6.23	99.39	110.60
1	A	94	ASN	CB-CA-C	6.04	122.48	110.40
1	A	193	LYS	CD-CE-NZ	5.87	125.20	111.70
1	A	123	GLU	CG-CD-OE1	-5.68	106.94	118.30
1	A	214	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	143	PHE	CB-CA-C	-5.27	99.86	110.40
1	A	72[A]	ARG	CA-CB-CG	5.24	124.93	113.40
1	A	72[B]	ARG	CA-CB-CG	5.24	124.93	113.40
1	B	149	GLU	CB-CA-C	5.16	120.71	110.40
1	B	211	GLN	CA-CB-CG	-5.14	102.09	113.40
1	A	12	LYS	CD-CE-NZ	-5.08	100.01	111.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	94	ASN	CA
1	A	227	LYS	CA
1	B	227	LYS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLU	Sidechain
1	A	143	PHE	Mainchain,Peptide
1	A	144	GLY	Mainchain,Peptide

## 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	1895	0	1865	26	0
1	B	1735	0	1736	17	0
2	A	24	0	12	0	0
2	B	24	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	195	0	0	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	188	0	0	11	0
All	All	4067	0	3625	39	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 6.

All (39) 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:B:217:THR:N	4:B:2178:HOH:O	1.96	0.97
1:B:189:ASP:HB2	4:B:2170:HOH:O	1.67	0.92
1:A:9:ASN:HB2	4:A:2011:HOH:O	1.85	0.77
1:A:144:GLY:O	4:A:2147:HOH:O	2.01	0.77
1:A:61:ASN:ND2	1:B:190:GLY:HA2	2.00	0.76
1:A:61:ASN:HB3	4:A:2070:HOH:O	1.93	0.69
1:B:88:GLU:C	4:B:2109:HOH:O	2.30	0.68
1:A:89:GLU:O	1:A:90:TYR:HB2	1.93	0.67
1:A:9:ASN:CB	4:A:2011:HOH:O	2.43	0.66
1:A:190:GLY:HA2	1:B:61:ASN:ND2	2.11	0.66
1:A:203:GLU:OE2	4:A:2182:HOH:O	2.14	0.64
1:B:61:ASN:ND2	4:B:2082:HOH:O	2.30	0.61
1:B:124:GLY:HA2	4:B:2126:HOH:O	2.00	0.61
1:A:61:ASN:HD21	1:B:190:GLY:HA2	1.66	0.60
1:A:190:GLY:HA2	1:B:61:ASN:HD21	1.67	0.59
1:A:144:GLY:CA	1:A:145:PHE:CB	2.86	0.53
1:A:144:GLY:CA	1:A:145:PHE:HB2	2.39	0.53
1:A:170:LYS:HD2	1:A:213:LEU:HD22	1.90	0.53
1:A:61:ASN:ND2	4:A:2071:HOH:O	2.38	0.52
1:A:9:ASN:ND2	1:A:169:TYR:OH	2.42	0.52
1:A:144:GLY:HA3	1:A:145:PHE:CB	2.40	0.52
1:A:208:ILE:O	1:A:211:GLN:HG2	2.12	0.50
1:B:124:GLY:CA	4:B:2126:HOH:O	2.57	0.50
4:A:2066:HOH:O	1:B:194:LYS:HE3	2.13	0.49
1:A:61:ASN:CB	4:A:2070:HOH:O	2.57	0.48
1:B:5:GLU:OE1	4:B:2006:HOH:O	2.20	0.48
1:B:67:ASN:C	1:B:67:ASN:HD22	2.17	0.47
1:B:40[A]:ARG:NH2	4:B:2047:HOH:O	2.44	0.46
1:A:72[B]:ARG:HD2	1:A:163:LEU:HG	1.96	0.46
1:B:97:ASP:N	4:B:2112:HOH:O	2.49	0.45
1:B:4:ILE:HD11	4:B:2118:HOH:O	2.16	0.45
1:A:112:GLN:H	1:A:112:GLN:HG3	1.61	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:NZ	1:A:213:LEU:HD13	2.33	0.43
1:A:40[A]:ARG:CZ	4:A:2044:HOH:O	2.67	0.42
1:A:40[B]:ARG:HD3	1:A:145:PHE:CD1	2.55	0.41
1:A:135:LEU:HG	1:A:139:LYS:HE2	2.03	0.41
1:A:123:GLU:HG3	4:A:2079:HOH:O	2.20	0.41
1:A:40[B]:ARG:NE	1:A:145:PHE:CD2	2.90	0.40
1:B:40[A]:ARG:NE	4:B:2047:HOH:O	2.48	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	226/229 (99%)	223 (99%)	1 (0%)	2 (1%)	17	4
1	B	203/229 (89%)	202 (100%)	1 (0%)	0	100	100
All	All	429/458 (94%)	425 (99%)	2 (0%)	2 (0%)	29	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PHE
1	A	145	PHE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/209 (100%)	207 (99%)	3 (1%)	67	46
1	B	191/209 (91%)	186 (97%)	5 (3%)	46	21
All	All	401/418 (96%)	393 (98%)	8 (2%)	55	32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	95	ASN
1	A	112	GLN
1	B	67	ASN
1	B	146	ASN
1	B	165	LEU
1	B	188	LYS
1	B	211	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	61	ASN
1	B	61	ASN
1	B	67	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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$
2	DUN	B	1230	3	25,25,25	2.72	10 (40%)	30,38,38	2.49	10 (33%)
2	DUN	A	1230	3	25,25,25	2.30	6 (24%)	30,38,38	1.87	7 (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
2	DUN	B	1230	3	-	1/13/28/28	0/2/2/2
2	DUN	A	1230	3	-	3/13/28/28	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1230	DUN	C6-N1	-6.45	1.35	1.47
2	B	1230	DUN	C6-N1	-6.24	1.36	1.47
2	A	1230	DUN	C6-C5	-6.08	1.36	1.52
2	B	1230	DUN	PA-O2A	5.89	1.55	1.46
2	B	1230	DUN	C6-C5	-5.45	1.38	1.52
2	B	1230	DUN	C5-C4	-5.18	1.38	1.50
2	A	1230	DUN	C5-C4	-4.01	1.40	1.50
2	A	1230	DUN	PA-O2A	3.10	1.51	1.46
2	B	1230	DUN	PB-O1B	-2.92	1.48	1.56
2	B	1230	DUN	PB-O2B	2.79	1.50	1.46
2	B	1230	DUN	C2-N1	2.45	1.39	1.35
2	B	1230	DUN	O2-C2	2.41	1.27	1.23
2	B	1230	DUN	C1'-N1	2.25	1.48	1.45
2	B	1230	DUN	PA-O1A	-2.22	1.50	1.56
2	A	1230	DUN	PA-N3A	2.21	1.69	1.63
2	A	1230	DUN	C2-N1	2.10	1.38	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1230	DUN	O2B-PB-N3A	-7.35	100.95	111.77
2	B	1230	DUN	O2A-PA-N3A	-5.79	103.24	111.77
2	B	1230	DUN	O1A-PA-O2A	4.48	119.32	109.92
2	B	1230	DUN	O2-C2-N1	-4.28	117.73	123.11
2	A	1230	DUN	O2-C2-N1	-4.27	117.75	123.11
2	A	1230	DUN	O1A-PA-O2A	4.07	118.46	109.92
2	A	1230	DUN	C5-C6-N1	3.62	123.55	111.61
2	B	1230	DUN	C4-N3-C2	-3.61	122.80	125.79
2	A	1230	DUN	O2A-PA-N3A	-3.59	106.48	111.77
2	A	1230	DUN	O2B-PB-N3A	-3.26	106.98	111.77
2	A	1230	DUN	O5'-PA-O2A	-3.08	102.41	114.24
2	B	1230	DUN	C5-C6-N1	3.03	121.61	111.61
2	B	1230	DUN	O4'-C1'-N1	2.86	112.06	108.41
2	B	1230	DUN	O5'-PA-O2A	-2.86	103.24	114.24
2	B	1230	DUN	C5-C4-N3	2.38	119.32	116.65
2	B	1230	DUN	O3B-PB-O1B	2.10	113.22	107.64
2	A	1230	DUN	O4'-C1'-N1	2.08	111.06	108.41

There are no chirality outliers.

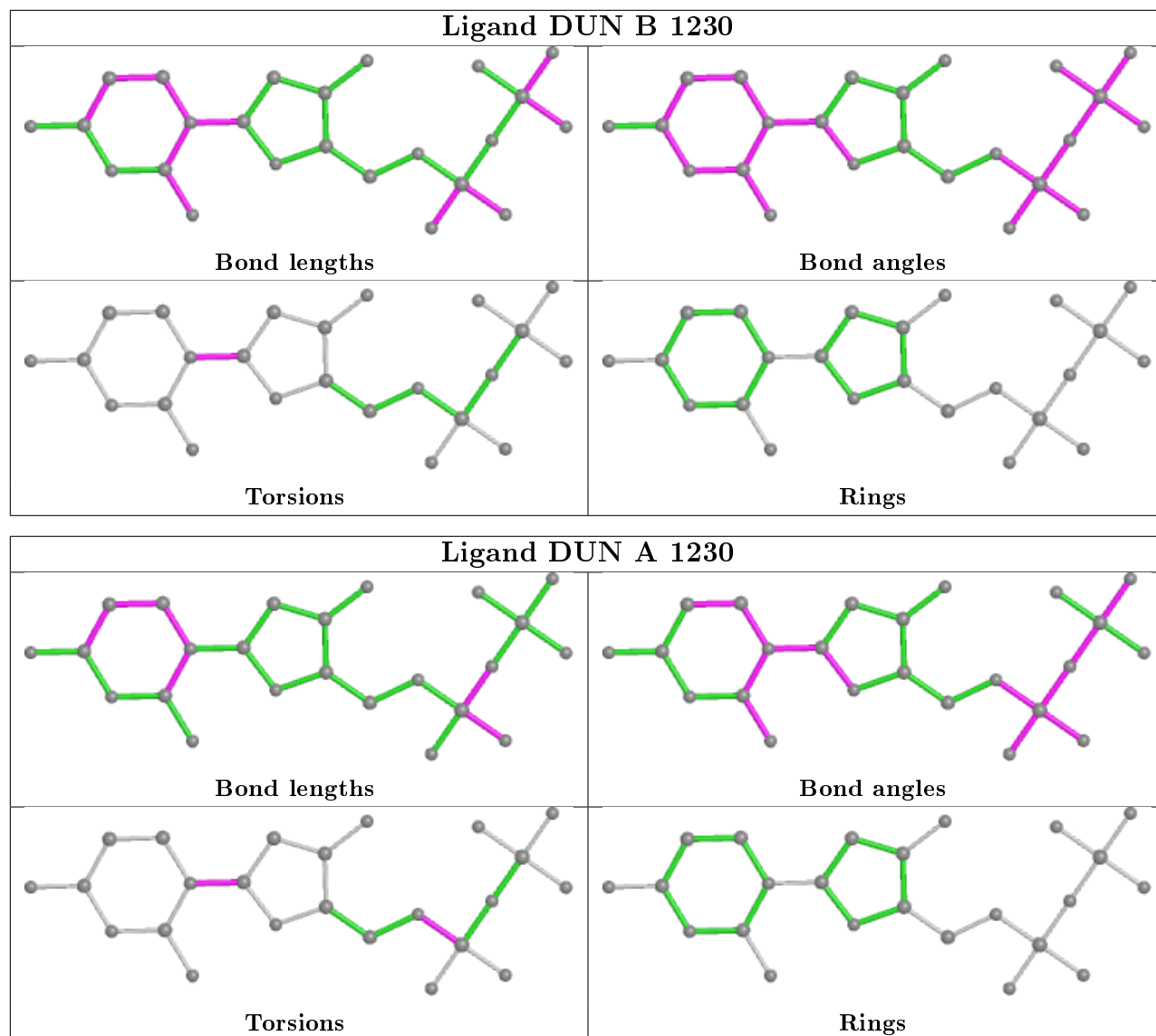
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1230	DUN	C5'-O5'-PA-O2A
2	A	1230	DUN	C5'-O5'-PA-O1A
2	A	1230	DUN	O4'-C1'-N1-C6
2	B	1230	DUN	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	143:PHE	C	144:GLY	N	1.01
1	A	144:GLY	C	145:PHE	N	0.98



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

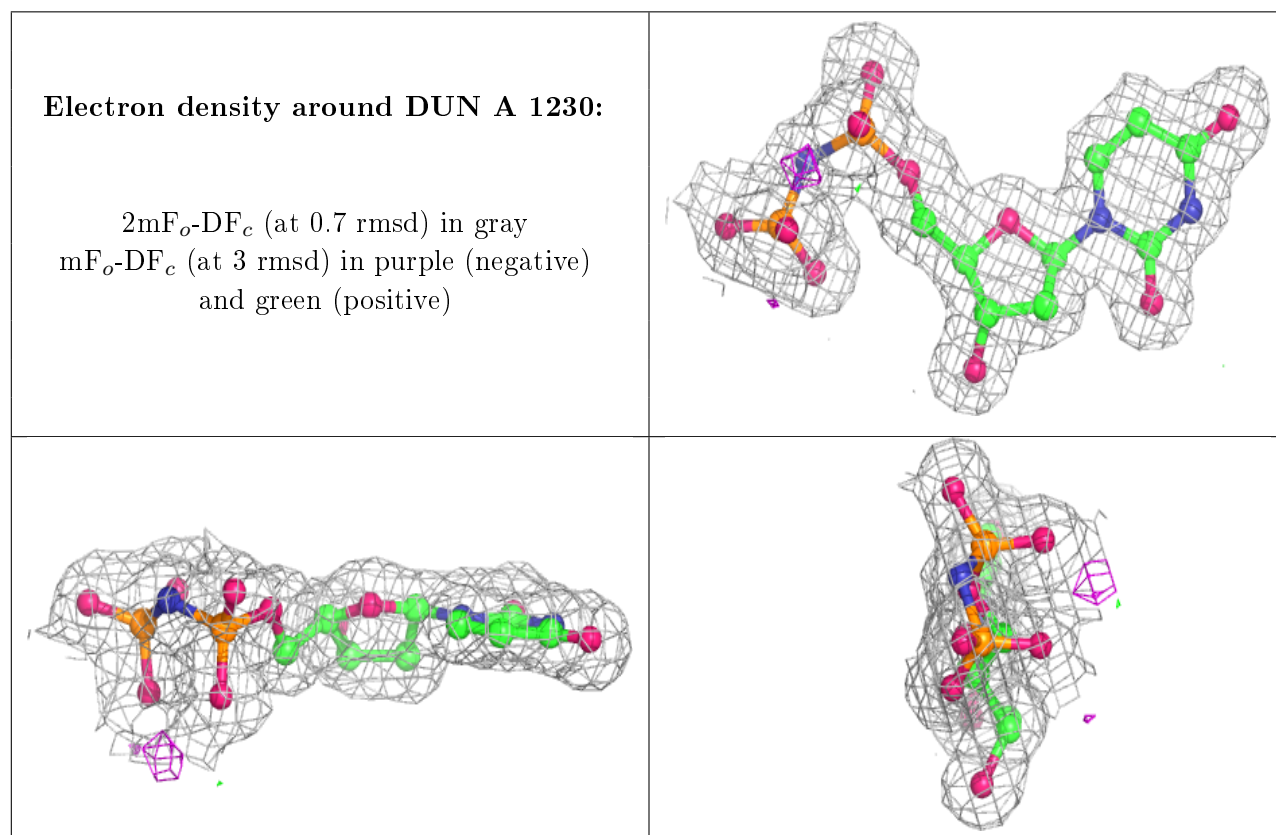
### 6.3 Carbohydrates ⓘ

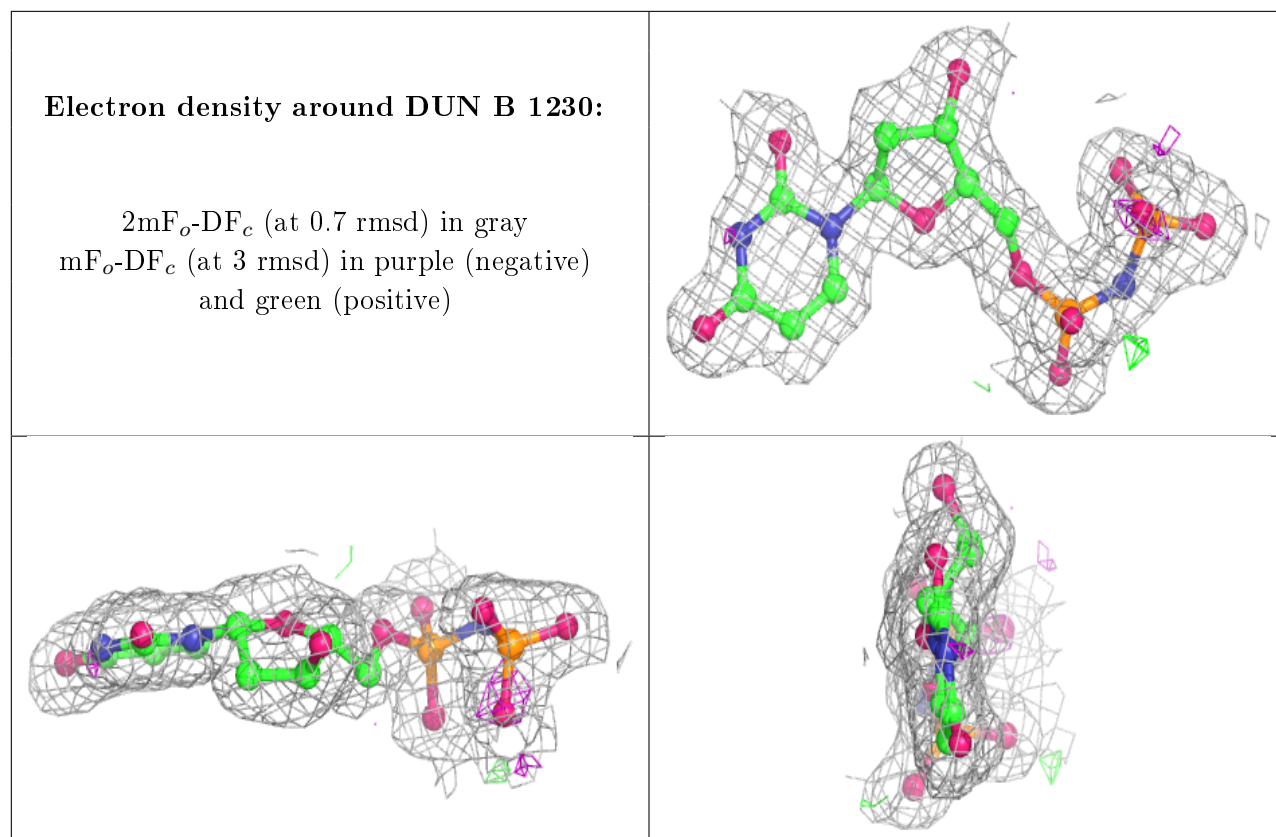
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.