



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:46 PM UTC

PDB ID : 3OSN / pdb_00003osn
Title : Structural Basis for Proficient Incorporation of dTTP Opposite O6-Methylguanine by Human DNA Polymerase Iota
Authors : Pence, M.G.
Deposited on : 2010-09-09
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

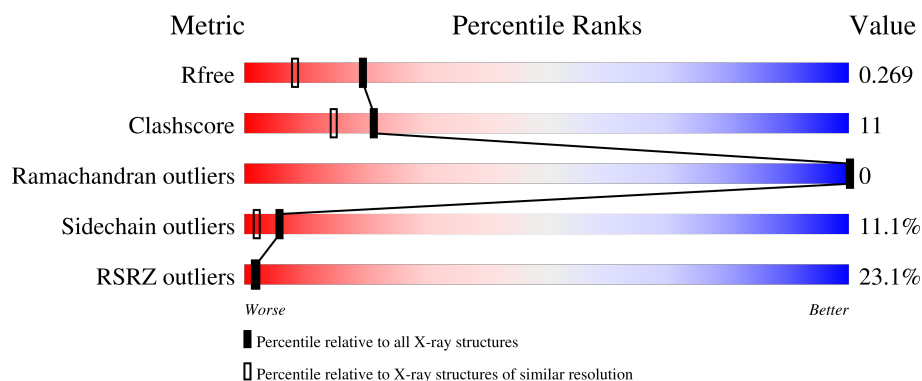
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	B	18	 22% 11% 6% 61%
1	C	18	 17% 17% 11% 56%
2	A	420	 22% 68% 17% 6% 8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

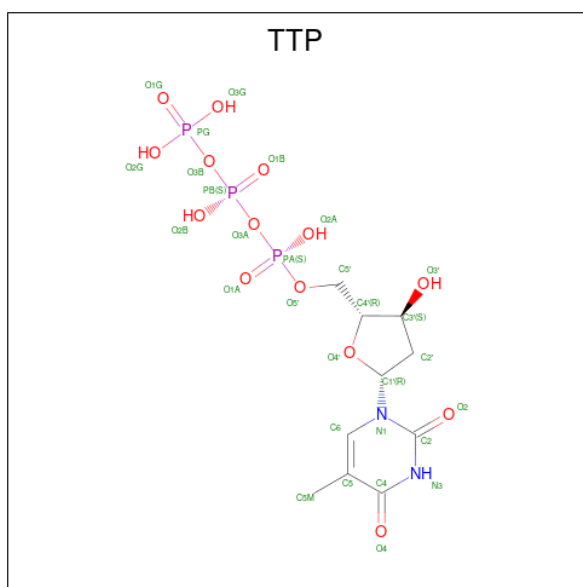
- Molecule 1 is a DNA chain called 5'-D(*TP*CP*TP*(6OG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	7	Total	C	N	O	P	0	0	0
			142	67	29	39	7			
1	C	8	Total	C	N	O	P	0	0	0
			167	79	30	50	8			

- Molecule 2 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	385	Total	C	N	O	S	0	0	0
			2999	1890	525	563	21			

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0

- Molecule 6 is water.

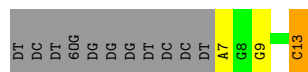
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	13	Total 13	O 13	0	0
6	C	19	Total 19	O 19	0	0
6	A	239	Total 239	O 239	0	0

3 Residue-property plots [i](#)

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

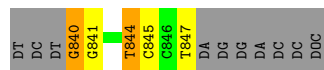
- Molecule 1: 5'-D(*TP*CP*TP*(6OG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain B: 



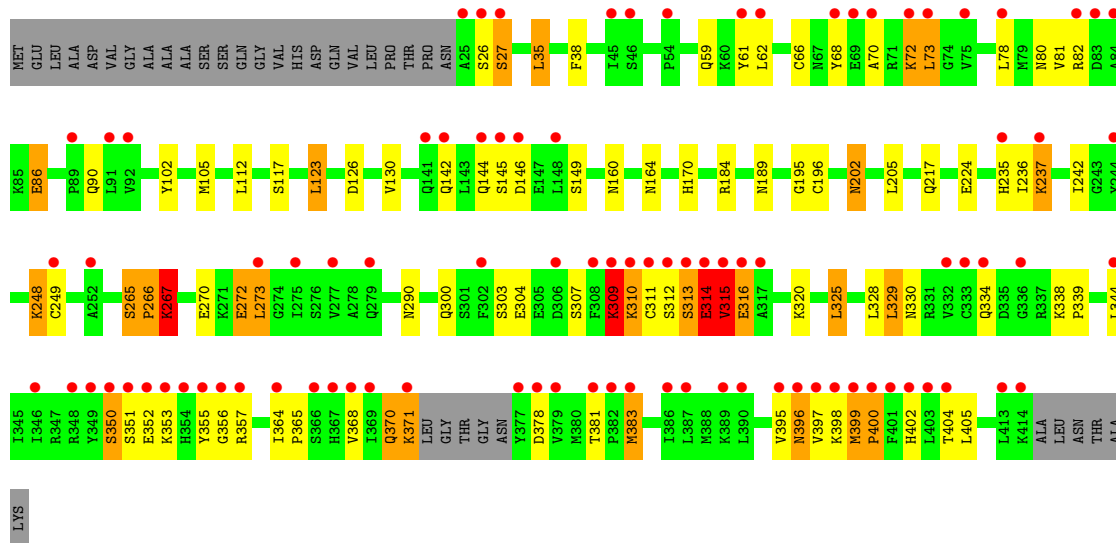
- Molecule 1: 5'-D(*TP*CP*TP*(6OG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain C: 



- Molecule 2: DNA polymerase iota

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.97Å 97.97Å 202.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.62 – 1.90 47.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.62-1.90) 99.5 (47.62-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.208 , 0.241 0.238 , 0.269	Depositor DCC
R_{free} test set	2327 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3611	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: MG, DOC, TTP, 6OG, NA

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	B	0.67	0/139	1.44	1/212 (0.5%)
1	C	0.83	0/160	1.54	1/245 (0.4%)
2	A	1.26	16/3040 (0.5%)	1.28	24/4101 (0.6%)
All	All	1.22	16/3339 (0.5%)	1.30	26/4558 (0.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	267	LYS	C-O	8.56	1.34	1.24
2	A	312	SER	CA-C	-7.46	1.45	1.53
2	A	242	ILE	CA-CB	7.18	1.62	1.53
2	A	267	LYS	C-N	7.17	1.43	1.33
2	A	265	SER	C-O	7.14	1.34	1.24
2	A	72	LYS	C-O	6.98	1.33	1.24
2	A	315	VAL	CA-CB	6.85	1.63	1.54
2	A	130	VAL	C-O	6.49	1.30	1.24
2	A	395	VAL	CA-CB	6.00	1.61	1.54
2	A	272	GLU	C-N	5.76	1.41	1.33
2	A	265	SER	C-N	5.64	1.42	1.33
2	A	123	LEU	C-O	-5.52	1.17	1.24
2	A	383	MET	CG-SD	5.49	1.94	1.80
2	A	381	THR	CA-CB	5.05	1.59	1.53
2	A	266	PRO	N-CD	5.04	1.54	1.47
2	A	273	LEU	C-N	5.01	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	GLU	N-CA-C	-11.96	98.18	113.72
2	A	314	GLU	N-CA-CB	10.66	128.62	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	311	CYS	N-CA-C	-9.98	100.64	112.92
2	A	146	ASP	N-CA-C	-9.88	99.01	112.94
2	A	355	TYR	N-CA-C	9.26	121.14	111.14
2	A	353	LYS	N-CA-C	8.24	128.36	110.80
2	A	400	PRO	N-CA-C	7.87	122.86	111.13
2	A	399	MET	CA-C-N	7.77	128.21	120.52
2	A	399	MET	C-N-CA	7.77	128.21	120.52
2	A	313	SER	N-CA-C	-7.52	95.20	108.13
2	A	313	SER	CB-CA-C	7.21	120.77	110.24
2	A	352	GLU	N-CA-C	-7.14	96.89	108.52
1	B	9	DG	O4'-C1'-N9	7.10	119.05	108.40
2	A	27	SER	N-CA-C	6.11	118.68	108.96
2	A	350	SER	N-CA-C	-5.68	95.10	111.00
2	A	356	GLY	N-CA-C	5.66	126.58	113.18
2	A	265	SER	O-C-N	5.50	126.09	121.31
2	A	312	SER	CA-C-O	5.47	127.84	120.89
2	A	312	SER	CA-C-N	5.43	130.44	121.86
2	A	312	SER	C-N-CA	5.43	130.44	121.86
1	C	844	DT	C2'-C3'-O3'	-5.22	103.67	111.50
2	A	309	LYS	CB-CA-C	-5.17	102.62	111.31
2	A	314	GLU	N-CA-C	-5.11	96.69	111.00
2	A	312	SER	N-CA-CB	5.07	120.59	111.36
2	A	102	TYR	N-CA-C	-5.05	105.86	111.36
2	A	38	PHE	N-CA-C	5.02	119.65	111.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	142	0	78	1	1
1	C	167	0	93	4	1
2	A	2999	0	3073	69	0
3	A	29	0	13	3	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	239	0	0	5	0
6	B	13	0	0	0	0
6	C	19	0	0	0	0
All	All	3611	0	3257	72	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 11.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:310:LYS:HE3	2:A:402:HIS:CB	1.67	1.23
2:A:399:MET:N	2:A:400:PRO:HD3	1.36	1.19
2:A:73:LEU:N	2:A:73:LEU:HD23	1.56	1.13
2:A:350:SER:CB	2:A:351:SER:HA	1.66	1.11
2:A:399:MET:N	2:A:400:PRO:CD	2.20	1.05
2:A:267:LYS:HD3	2:A:267:LYS:H	1.15	1.03
2:A:398:LYS:C	2:A:400:PRO:HD3	1.86	1.01
2:A:350:SER:HB3	2:A:351:SER:HA	1.00	1.00
2:A:144:GLN:O	2:A:145:SER:OG	1.80	0.99
2:A:310:LYS:CE	2:A:402:HIS:CB	2.41	0.99
2:A:249:CYS:HB2	6:A:644:HOH:O	1.62	0.98
2:A:350:SER:HB3	2:A:351:SER:CA	1.95	0.96
2:A:73:LEU:N	2:A:73:LEU:CD2	2.30	0.93
2:A:315:VAL:O	2:A:315:VAL:HG13	1.69	0.93
2:A:164:ASN:H	2:A:170:HIS:HD2	1.11	0.91
2:A:290:ASN:HB2	6:A:560:HOH:O	1.71	0.91
2:A:72:LYS:C	2:A:73:LEU:HD23	2.04	0.82
2:A:267:LYS:HD3	2:A:267:LYS:N	1.93	0.80
2:A:164:ASN:H	2:A:170:HIS:CD2	2.01	0.75
2:A:399:MET:H	2:A:400:PRO:HD3	1.46	0.75
2:A:189:ASN:HB3	6:A:626:HOH:O	1.85	0.75
2:A:144:GLN:C	2:A:145:SER:HG	1.89	0.73
2:A:267:LYS:H	2:A:267:LYS:CD	1.97	0.72
2:A:316:GLU:O	2:A:320:LYS:HG2	1.89	0.72
2:A:73:LEU:HD23	2:A:73:LEU:H	1.57	0.69
2:A:35:LEU:HD12	2:A:195:GLY:HA3	1.74	0.69
2:A:315:VAL:O	2:A:315:VAL:CG1	2.41	0.68
2:A:350:SER:CB	2:A:351:SER:CA	2.58	0.62
2:A:105:MET:HE1	6:A:524:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:ASN:HD22	2:A:202:ASN:C	2.10	0.59
2:A:396:ASN:O	2:A:396:ASN:ND2	2.30	0.58
2:A:112:LEU:C	2:A:112:LEU:HD23	2.28	0.58
2:A:325:LEU:CD1	2:A:329:LEU:HD22	2.33	0.57
1:C:844:DT:H2''	1:C:845:DC:H5'	1.85	0.57
2:A:202:ASN:ND2	2:A:205:LEU:H	2.02	0.56
1:C:841:DG:OP2	2:A:307:SER:HB2	2.10	0.52
2:A:310:LYS:HE2	2:A:402:HIS:CB	2.35	0.50
2:A:304:GLU:HG3	2:A:328:LEU:HG	1.93	0.49
2:A:235:HIS:CE1	2:A:237:LYS:HE3	2.48	0.49
2:A:316:GLU:HA	2:A:316:GLU:OE1	2.13	0.48
2:A:68:TYR:O	2:A:72:LYS:HG3	2.13	0.48
2:A:371:LYS:N	2:A:371:LYS:HD3	2.29	0.48
2:A:398:LYS:C	2:A:400:PRO:CD	2.70	0.48
2:A:300:GLN:NE2	6:A:639:HOH:O	2.46	0.47
2:A:309:LYS:HD3	2:A:309:LYS:HA	1.54	0.47
2:A:72:LYS:C	2:A:73:LEU:CD2	2.81	0.47
1:C:840:6OG:H8	2:A:59:GLN:OE1	2.15	0.46
2:A:266:PRO:O	2:A:270:GLU:HG3	2.16	0.46
2:A:370:GLN:HA	2:A:370:GLN:OE1	2.14	0.46
2:A:61:TYR:CD1	2:A:61:TYR:N	2.84	0.46
2:A:235:HIS:ND1	2:A:237:LYS:HE3	2.31	0.45
2:A:314:GLU:O	2:A:315:VAL:HG12	2.16	0.45
2:A:196:CYS:HA	2:A:217:GLN:O	2.17	0.45
2:A:90:GLN:OE1	2:A:90:GLN:N	2.30	0.44
1:B:13:DOC:H2'	3:A:421:TTP:C6	2.53	0.44
2:A:267:LYS:N	2:A:267:LYS:CD	2.67	0.44
2:A:365:PRO:HB2	2:A:368:VAL:HG23	1.99	0.44
2:A:237:LYS:HB3	2:A:237:LYS:HE2	1.88	0.43
2:A:249:CYS:SG	2:A:273:LEU:HD21	2.57	0.43
2:A:396:ASN:ND2	2:A:400:PRO:HA	2.32	0.43
2:A:126:ASP:OD1	3:A:421:TTP:O5'	2.36	0.43
2:A:184:ARG:HD2	2:A:195:GLY:O	2.19	0.43
2:A:82:ARG:O	2:A:86:GLU:HB2	2.19	0.43
2:A:61:TYR:C	2:A:81:VAL:HG23	2.45	0.42
2:A:202:ASN:C	2:A:202:ASN:ND2	2.78	0.42
2:A:66:CYS:HB2	2:A:70:ALA:HB3	2.02	0.42
1:C:840:6OG:O6	3:A:421:TTP:O4	2.39	0.41
2:A:303:SER:O	2:A:304:GLU:HG2	2.20	0.41
2:A:338:LYS:HA	2:A:339:PRO:HD3	1.90	0.41
2:A:364:ILE:HD13	2:A:383:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:248:LYS:HD3	2:A:248:LYS:HA	1.88	0.40
2:A:170:HIS:HE1	2:A:224:GLU:OE2	2.04	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)
1:B:7:DA:P	1:C:847:DT:O3'[10_665]	1.92	0.28

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	
2	A	381/420 (91%)	369 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	342/376 (91%)	304 (89%)	38 (11%)	6	2

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	26	SER
2	A	27	SER
2	A	35	LEU
2	A	62	LEU
2	A	73	LEU
2	A	78	LEU
2	A	80	ASN
2	A	86	GLU
2	A	117	SER
2	A	123	LEU
2	A	142	GLN
2	A	149	SER
2	A	160	ASN
2	A	202	ASN
2	A	236	ILE
2	A	237	LYS
2	A	248	LYS
2	A	265	SER
2	A	267	LYS
2	A	272	GLU
2	A	309	LYS
2	A	310	LYS
2	A	313	SER
2	A	314	GLU
2	A	315	VAL
2	A	325	LEU
2	A	329	LEU
2	A	330	ASN
2	A	334	GLN
2	A	344	LEU
2	A	357	ARG
2	A	370	GLN
2	A	371	LYS
2	A	378	ASP
2	A	396	ASN
2	A	397	VAL
2	A	404	THR
2	A	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	58	GLN

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Mol	Chain	Res	Type
2	A	128	ASN
2	A	144	GLN
2	A	159	ASN
2	A	170	HIS
2	A	202	ASN
2	A	262	GLN
2	A	282	GLN
2	A	290	ASN
2	A	300	GLN
2	A	330	ASN
2	A	334	GLN
2	A	361	GLN
2	A	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	DOC	B	13	1	16,19,20	1.83	4 (25%)	20,26,29	2.15	2 (10%)
1	6OG	C	840	-	22,25,26	1.74	6 (27%)	31,36,39	5.13	13 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DOC	B	13	1	-	0/7/18/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6OG	C	840	-	-	0/9/23/24	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	DOC	O4'-C1'	4.09	1.51	1.42
1	C	840	6OG	C5-N7	-3.77	1.32	1.39
1	C	840	6OG	O4'-C1'	3.66	1.50	1.42
1	B	13	DOC	C4-N3	3.60	1.41	1.34
1	C	840	6OG	C5-C6	-3.43	1.35	1.41
1	B	13	DOC	C6-C5	2.97	1.42	1.35
1	C	840	6OG	C5'-C4'	2.76	1.59	1.51
1	C	840	6OG	C4-N9	-2.07	1.33	1.37
1	B	13	DOC	C6-N1	2.04	1.42	1.38
1	C	840	6OG	C5-C4	-2.04	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	840	6OG	C-O6-C6	-21.71	96.90	117.20
1	C	840	6OG	C5-C4-N3	-9.26	117.42	127.18
1	C	840	6OG	N3-C4-N9	8.59	137.90	126.99
1	B	13	DOC	O4'-C4'-C5'	-7.39	96.01	109.34
1	C	840	6OG	C6-C5-N7	-6.97	125.64	133.82
1	C	840	6OG	C4-C5-C6	5.92	121.03	115.22
1	C	840	6OG	O4'-C1'-N9	-5.24	98.55	107.96
1	B	13	DOC	C4'-O4'-C1'	-4.16	105.88	109.81
1	C	840	6OG	O6-C6-N1	3.65	123.82	118.96
1	C	840	6OG	N9-C8-N7	-3.15	109.47	113.94
1	C	840	6OG	O6-C6-C5	-2.56	114.09	117.17
1	C	840	6OG	C2-N3-C4	2.46	120.10	113.51
1	C	840	6OG	C4-C5-N7	2.39	113.32	110.58
1	C	840	6OG	O4'-C4'-C5'	2.30	116.71	109.33
1	C	840	6OG	C4-N9-C8	2.19	108.04	105.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	13	DOC	1	0
1	C	840	6OG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
3	TTP	A	421	4	29,30,30	3.19	10 (34%)	43,47,47	3.14	18 (41%)

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	TTP	A	421	4	-	7/22/34/34	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	421	TTP	PB-O3B	10.47	1.70	1.59
3	A	421	TTP	PB-O3A	7.64	1.67	1.59
3	A	421	TTP	O3'-C3'	6.07	1.56	1.43
3	A	421	TTP	C2'-C1'	4.08	1.63	1.52
3	A	421	TTP	C4-C5	-3.80	1.38	1.44
3	A	421	TTP	C6-C5	3.78	1.40	1.34
3	A	421	TTP	PB-O1B	3.61	1.63	1.50
3	A	421	TTP	O4'-C4'	2.58	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	421	TTP	C6-N1	2.43	1.42	1.38
3	A	421	TTP	C2'-C3'	2.27	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	421	TTP	O4'-C1'-N1	-9.05	91.81	107.86
3	A	421	TTP	C5-C4-N3	7.11	121.50	115.32
3	A	421	TTP	C5'-C4'-C3'	-6.59	77.78	114.64
3	A	421	TTP	C4-N3-C2	-5.92	119.58	127.34
3	A	421	TTP	O3B-PB-O1B	5.50	127.24	110.70
3	A	421	TTP	O4-C4-C5	-4.74	119.50	124.92
3	A	421	TTP	N3-C2-N1	4.34	120.54	114.89
3	A	421	TTP	C5-C6-N1	-4.34	118.60	123.31
3	A	421	TTP	O2B-PB-O3A	-4.22	95.87	107.27
3	A	421	TTP	O4'-C4'-C5'	-3.94	96.70	109.33
3	A	421	TTP	O3G-PG-O2G	-3.19	95.82	107.80
3	A	421	TTP	O4'-C4'-C3'	3.11	112.75	105.65
3	A	421	TTP	O2B-PB-O3B	-3.10	98.89	107.27
3	A	421	TTP	O2-C2-N1	-2.80	119.15	122.80
3	A	421	TTP	O3B-PG-O1G	2.73	125.40	111.04
3	A	421	TTP	O3'-C3'-C2'	2.60	119.91	110.88
3	A	421	TTP	O3A-PA-O1A	-2.46	103.30	110.70
3	A	421	TTP	O2A-PA-O1A	2.16	122.47	112.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

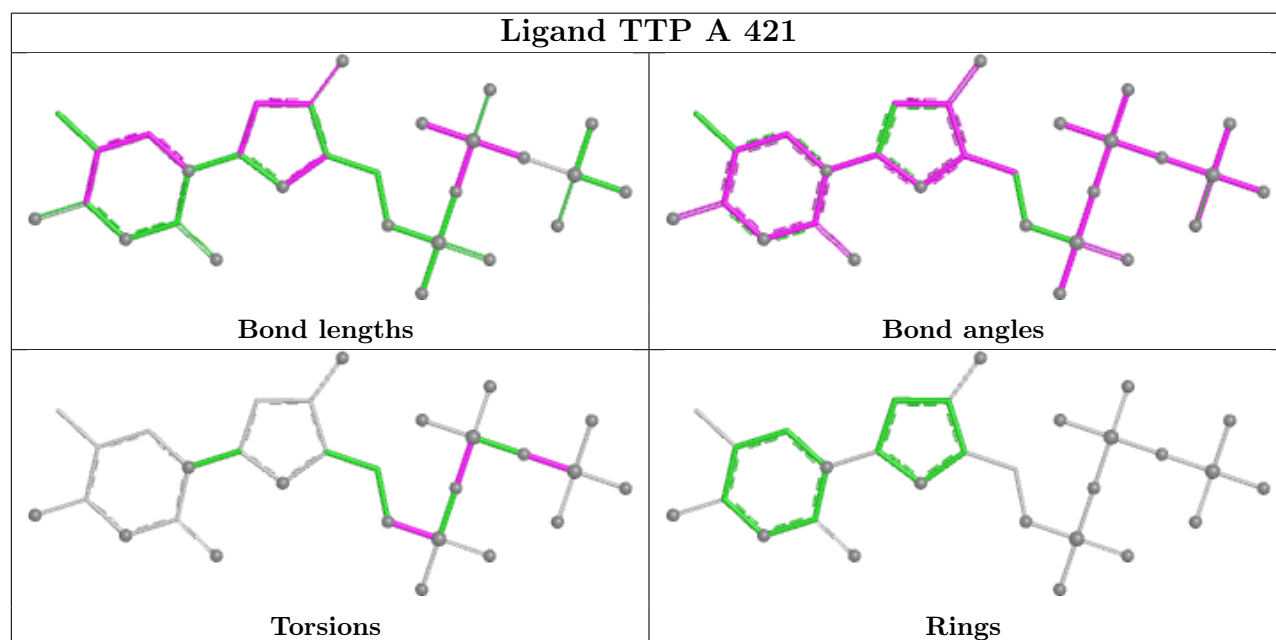
Mol	Chain	Res	Type	Atoms
3	A	421	TTP	C5'-O5'-PA-O2A
3	A	421	TTP	PB-O3B-PG-O2G
3	A	421	TTP	PA-O3A-PB-O1B
3	A	421	TTP	C5'-O5'-PA-O1A
3	A	421	TTP	C5'-O5'-PA-O3A
3	A	421	TTP	PB-O3B-PG-O1G
3	A	421	TTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	421	TTP	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	B	6/18 (33%)	0.11	0	100 100	34, 50, 57, 59	0
1	C	7/18 (38%)	-0.33	0	100 100	29, 33, 45, 59	0
2	A	385/420 (91%)	1.15	92 (23%)	2 1	20, 47, 120, 168	0
All	All	398/456 (87%)	1.11	92 (23%)	2 2	20, 47, 120, 168	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	315	VAL	8.2
2	A	401	PHE	6.6
2	A	311	CYS	6.2
2	A	399	MET	5.9
2	A	349	TYR	5.9
2	A	354	HIS	5.6
2	A	25	ALA	5.3
2	A	355	TYR	5.0
2	A	397	VAL	4.9
2	A	350	SER	4.7
2	A	78	LEU	4.4
2	A	400	PRO	4.3
2	A	313	SER	4.1
2	A	379	VAL	4.1
2	A	69	GLU	4.0
2	A	353	LYS	3.9
2	A	309	LYS	3.9
2	A	334	GLN	3.8
2	A	145	SER	3.7
2	A	332	VAL	3.6
2	A	351	SER	3.6
2	A	377	TYR	3.3
2	A	73	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	310	LYS	3.3
2	A	404	THR	3.3
2	A	89	PRO	3.2
2	A	148	LEU	3.1
2	A	249	CYS	3.1
2	A	275	ILE	3.1
2	A	92	VAL	3.1
2	A	395	VAL	3.1
2	A	306	ASP	3.0
2	A	75	VAL	3.0
2	A	244	TYR	3.0
2	A	333	CYS	3.0
2	A	413	LEU	3.0
2	A	277	VAL	2.9
2	A	356	GLY	2.9
2	A	389	LYS	2.9
2	A	308	PHE	2.9
2	A	364	ILE	2.9
2	A	61	TYR	2.9
2	A	378	ASP	2.8
2	A	273	LEU	2.8
2	A	316	GLU	2.8
2	A	352	GLU	2.8
2	A	371	LYS	2.8
2	A	383	MET	2.8
2	A	72	LYS	2.7
2	A	252	ALA	2.7
2	A	357	ARG	2.7
2	A	91	LEU	2.6
2	A	386	ILE	2.6
2	A	312	SER	2.6
2	A	396	ASN	2.6
2	A	62	LEU	2.5
2	A	144	GLN	2.5
2	A	382	PRO	2.5
2	A	146	ASP	2.5
2	A	54	PRO	2.5
2	A	336	GLY	2.4
2	A	68	TYR	2.4
2	A	235	HIS	2.4
2	A	390	LEU	2.4
2	A	402	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	142	GLN	2.4
2	A	237	LYS	2.4
2	A	83	ASP	2.4
2	A	367	HIS	2.4
2	A	82	ARG	2.4
2	A	141	GLN	2.4
2	A	346	ILE	2.4
2	A	344	LEU	2.3
2	A	45	ILE	2.3
2	A	70	ALA	2.3
2	A	84	ALA	2.3
2	A	368	VAL	2.3
2	A	26	SER	2.3
2	A	381	THR	2.2
2	A	302	PHE	2.2
2	A	369	ILE	2.2
2	A	348	ARG	2.2
2	A	403	LEU	2.2
2	A	279	GLN	2.1
2	A	46	SER	2.1
2	A	414	LYS	2.1
2	A	387	LEU	2.1
2	A	27	SER	2.0
2	A	366	SER	2.0
2	A	317	ALA	2.0
2	A	314	GLU	2.0
2	A	398	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	6OG	C	840	23/24	0.86	0.13	28,37,49,50	0
1	DOC	B	13	18/19	0.98	0.05	30,31,34,34	0

6.3 Carbohydrates [i](#)

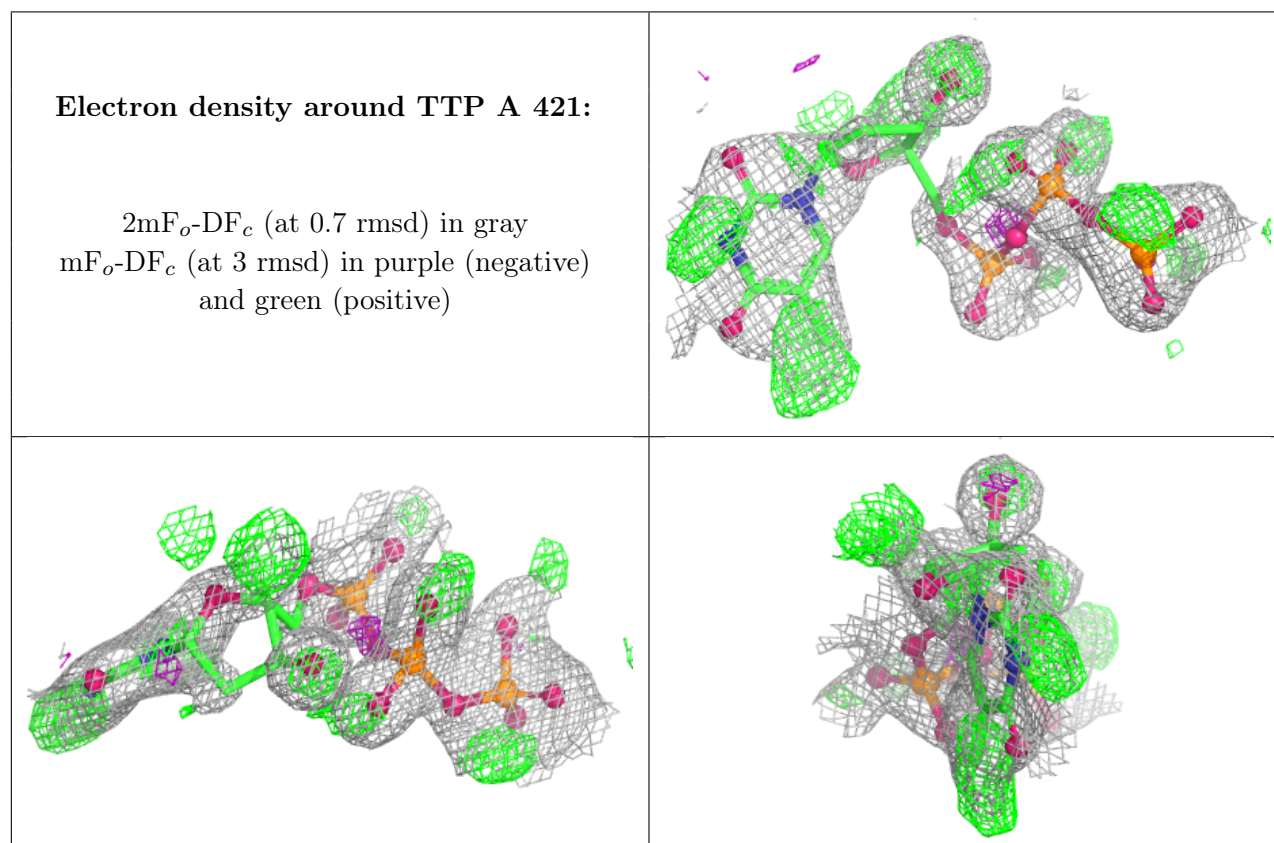
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	MG	A	424	1/1	0.67	0.24	30,30,30,30	1
3	TTP	A	421	29/29	0.84	0.19	12,33,38,44	25
4	MG	A	422	1/1	0.92	0.09	31,31,31,31	1
5	NA	A	423	1/1	0.94	0.07	34,34,34,34	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.