



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:12 AM UTC

PDB ID : 9ICC / pdb_00009icc
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + 2'-DEOXY ADENOSINE-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DATP AND CRCL3
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

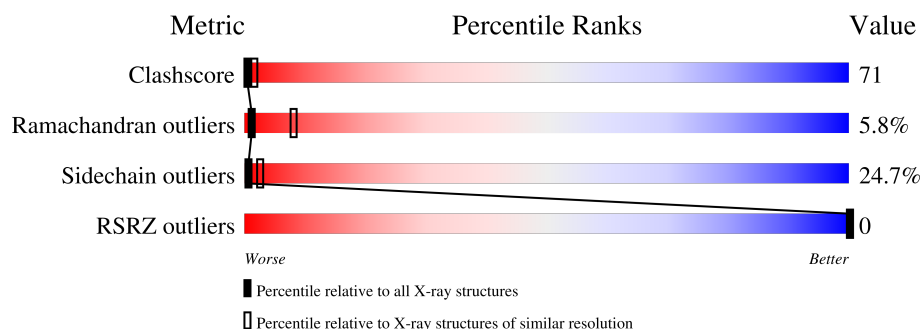
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	T	8	25% 75%
2	P	7	29% 71%
3	A	335	17% 43% 32% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	26	0	0
			2623	1657	458	499	9			

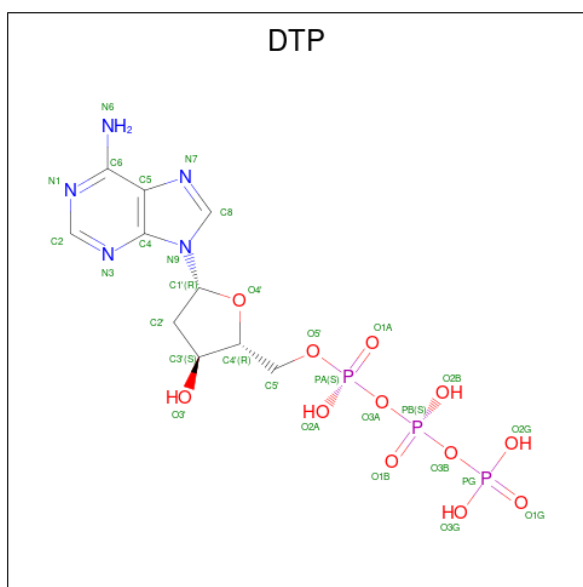
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHROMIUM ION (CCD ID: CR) (formula: Cr).

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

- Molecule 6 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			20	5	12	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	14	Total O 14 14	0	0
7	P	19	Total O 19 19	0	0
7	A	108	Total O 108 108	0	0

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 (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')

Chain T: 

C1 A2 T3 T4 A5 A6 A7 A8

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

Chain P: 

T1 C2 T3 A4 A5 T6 G7

- Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))

Chain A: 

MET SER ARG LYS LYS ALA PRG GLN E9 T10 T11 T12 T13 T14 T15 T16 T17 T18 T19 T20 T21 T22 T23 T24 T25 T26 T27 T28 T29 T30 T31 T32 T33 T34 T35 T36 T37 T38 T39 T40 T41 T42 T43 T44 T45 T46 T47 T48 T49 T50 T51 T52 T53 T54 T55 T56 T57 T58 T59 T60 T61 T62 T63 T64 T65 T66 T67 T68 T69 T70 T71 T72 T73 T74 T75 T76 T77 T78 T79 T80 T81 T82 T83 T84 T85 T86 T87 T88 T89 T90 T91 T92 T93 T94 T95 T96 T97 T98 T99 T100 T101 T102 T103 T104 T105 T106 T107 T108 T109 T110 T111 T112 T113 T114 T115 T116 T117 T118 T119 T120 T121 T122 T123 T124

P63 G64 V65 G66 G67 G68 G69 G70 G71 G72 G73 G74 G75 G76 G77 G78 G79 G80 G81 G82 G83 G84 G85 G86 G87 G88 G89 G90 G91 G92 G93 G94 G95 G96 G97 G98 G99 G100 G101 G102 G103 G104 G105 G106 G107 G108 G109 G110 G111 G112 G113 G114 G115 G116 G117 G118 G119 G120 G121 G122 G123 G124

L125 R126 K127 N128 N129 D130 K131 L132 L133 L134 L135 L136 L137 L138 L139 L140 L141 L142 L143 L144 L145 L146 L147 L148 L149 L150 L151 L152 L153 L154 L155 L156 L157 L158 L159 L160 L161 L162 L163 L164 L165 L166 L167 L168 L169 L170 L171 L172 L173 L174 L175 L176 L177 L178 L179 L180 L181 L182 L183 L184

A185 E186 S187 S188 G189 D190 L191 L192 L193 L194 L195 L196 L197 L198 L199 L200 L201 L202 L203 L204 L205 L206 L207 L208 L209 L210 L211 L212 L213 L214 L215 L216 L217 L218 L219 L220 L221 L222 L223 L224 L225 L226 L227 L228 L229 L230 L231 L232 L233 L234 L235 L236 L237 L238 L239 L240 L241 L242 L243 L244 L245 L246

E247 K248 E249 Y250 P251 D252 H253 R254 R255 R256 L259 L260 P261 K262 Q263 Q264 Y265 Y266 C267 K268 V269 P270 L271 Y272 F273 T274 S275 T276 T277 T278 T279 K280 N281 M282 R283 A286 L287 E288 K289 G290 G291 T292 T293 N294 Y296 Y297 T298 R299 P300 L301 G302 G303 T304 G305 V306 A307 G308

E309 P310 E311 P312 V313 D314 H315 S316 E317 K318 L319 F320 D321 Y322 L323 Q324 W325 K326 Y327 R328 E329 P330 K331 R332 R333 S334 E335

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.30Å 57.60Å 48.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.10) 91.6 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	6.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.158 , (Not available) 0.154 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 119.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3076	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: DTP, NA, CR

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	T	1.08	0/162	3.63	16/249 (6.4%)
2	P	1.16	1/160 (0.6%)	3.82	16/243 (6.6%)
3	A	1.62	17/2672 (0.6%)	2.23	128/3590 (3.6%)
All	All	1.57	18/2994 (0.6%)	2.46	160/4082 (3.9%)

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
3	A	4	0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	242	PRO	N-CA	-7.43	1.38	1.47
3	A	242	PRO	CA-C	-7.38	1.43	1.52
3	A	36	TYR	N-CA	-7.20	1.37	1.46
3	A	196	THR	CA-C	-6.67	1.44	1.52
3	A	241	LEU	CA-C	-6.66	1.45	1.52

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-24.95	89.63	127.05
2	P	7	DG	C8-N9-C1'	24.11	163.17	127.00
1	T	7	DA	C8-N9-C1'	23.93	162.94	127.05
2	P	7	DG	C4-N9-C1'	-23.61	91.58	127.00
1	T	4	DT	C6-N1-C1'	-20.64	88.39	119.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	12	ASN	CA
3	A	205	THR	CA
3	A	246	ASP	CA
3	A	309	GLU	CA

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	T	145	0	80	11	0
2	P	144	0	81	15	0
3	A	2623	0	2641	379	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	20	0	7	4	0
7	A	108	0	0	17	0
7	P	19	0	0	2	0
7	T	14	0	0	2	0
All	All	3076	0	2809	401	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 71.

The worst 5 of 401 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)
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.41	1.02
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.39	1.01
2:P:1:DT:H2''	2:P:2:DC:H5'	1.41	1.01
3:A:245:ASN:N	3:A:245:ASN:HD22	1.55	0.99
2:P:5:DA:H2''	2:P:6:DT:H5'	1.45	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	259 (80%)	47 (14%)	19 (6%)	1 8

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	80	GLY
3	A	185	ALA
3	A	204	SER
3	A	205	THR
3	A	206	LYS

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
3	A	288/295 (98%)	217 (75%)	71 (25%)	1 2

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	292	THR
3	A	294	ASN
3	A	311	LEU
3	A	121	THR
3	A	119	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	279	ASN
3	A	264	GLN
3	A	159	GLN
3	A	252	HIS
3	A	157	GLN

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 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	$\# Z > 2$
6	DTP	A	338	5	19,20,32	2.73	5 (26%)	25,31,50	1.63	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTP	A	338	5	-	2/18/28/34	0/1/1/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DTP	PA-O3A	-7.95	1.50	1.59
6	A	338	DTP	PB-O3B	-6.32	1.52	1.59
6	A	338	DTP	PB-O3A	-3.18	1.56	1.59
6	A	338	DTP	O5'-C5'	-2.37	1.35	1.44
6	A	338	DTP	PB-O2B	-2.33	1.44	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DTP	O3A-PB-O1B	-4.01	98.63	110.70
6	A	338	DTP	O2B-PB-O3A	3.88	117.76	107.27
6	A	338	DTP	O2B-PB-O3B	3.36	116.35	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	DTP	O4'-C4'-C5'-O5'
6	A	338	DTP	PB-O3B-PG-O3G

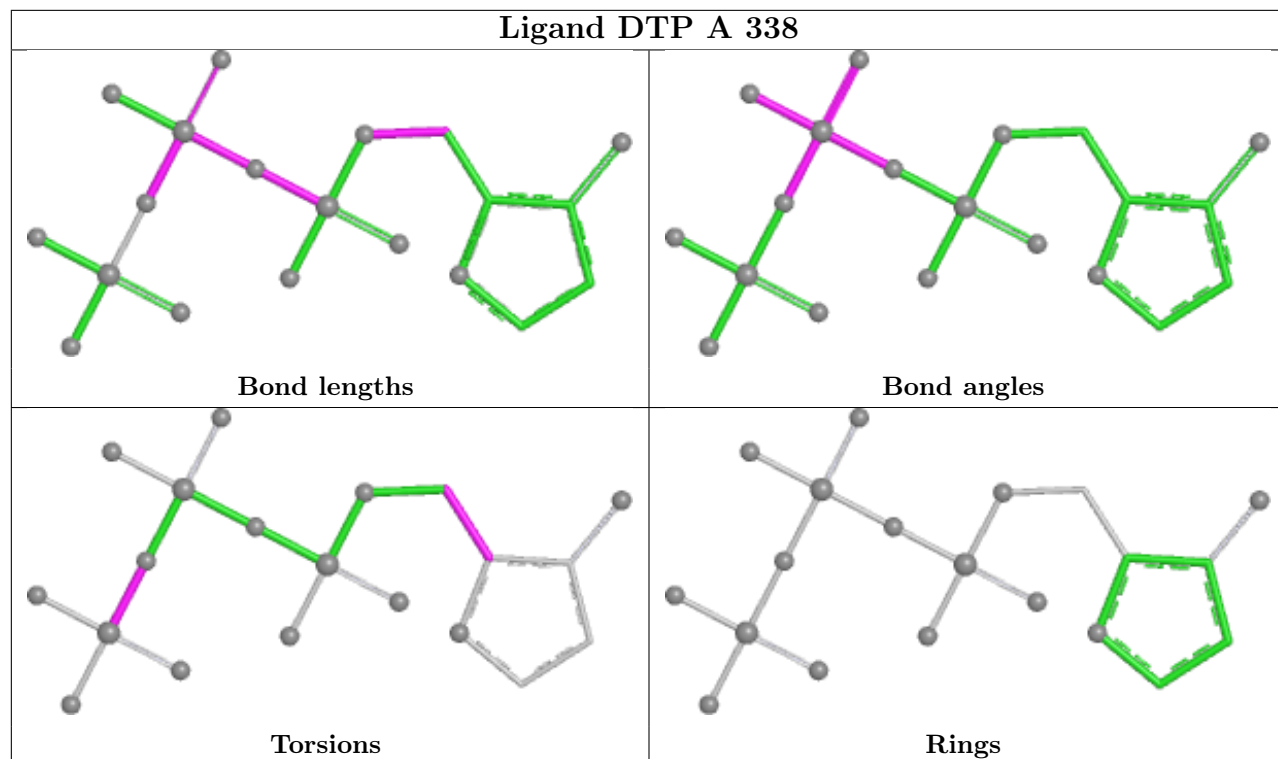
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	DTP	4	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	T	8/8 (100%)	-0.66	0 100 100	12, 46, 99, 100	0
2	P	7/7 (100%)	-1.02	0 100 100	23, 27, 43, 74	0
3	A	324/335 (96%)	-1.01	0 100 100	4, 36, 86, 100	0
All	All	339/350 (96%)	-1.00	0 100 100	4, 36, 87, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

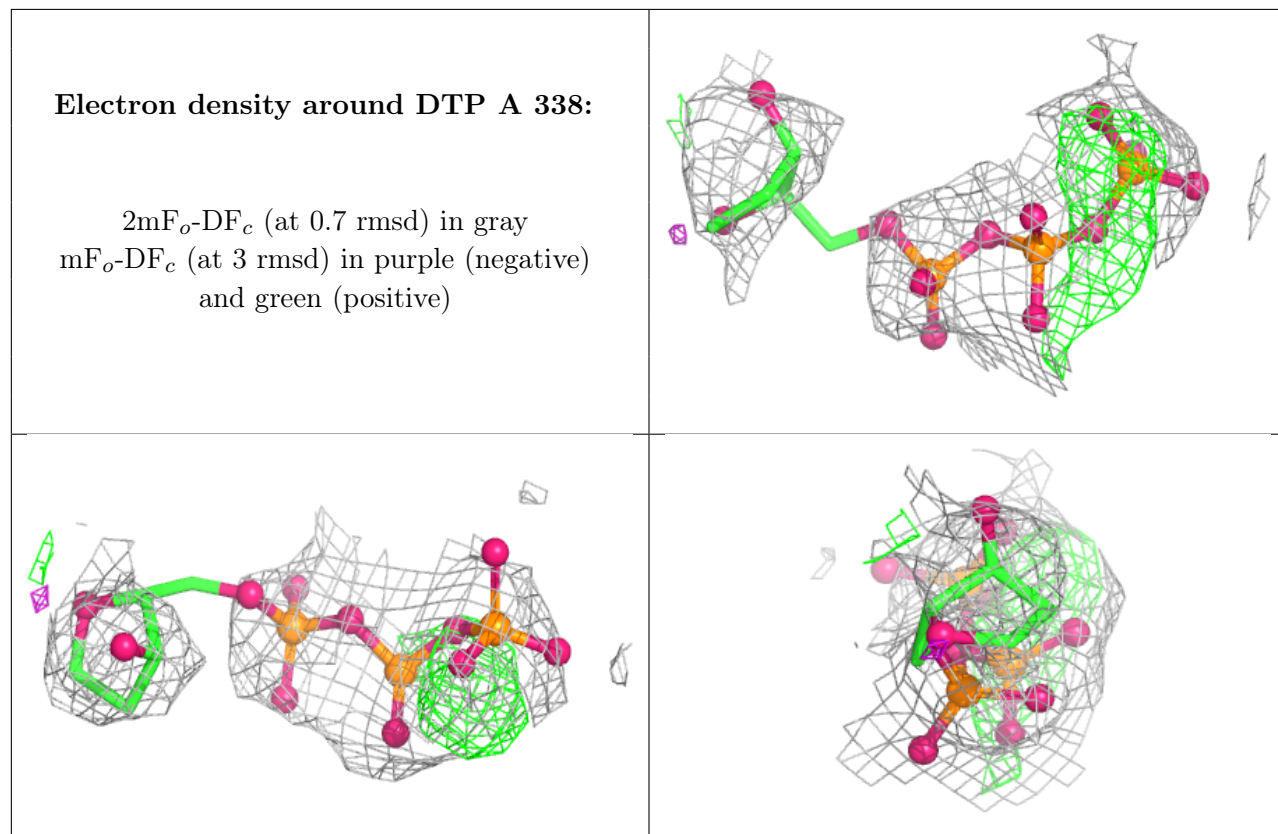
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
6	DTP	A	338	20/30	0.89	0.15	30,60,84,85	20
4	NA	A	341	1/1	0.93	0.01	12,12,12,12	0
4	NA	A	342	1/1	0.94	0.05	35,35,35,35	0
5	CR	A	339	1/1	0.96	0.04	30,30,30,30	1

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.