



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:46 AM UTC

PDB ID : 8B77 / pdb_00008b77
Title : The crystal structure of N828V variant of DNA Pol Epsilon containing dATP in the polymerase active site
Authors : Parkash, V.; Johansson, E.
Deposited on : 2022-09-29
Resolution : 2.70 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

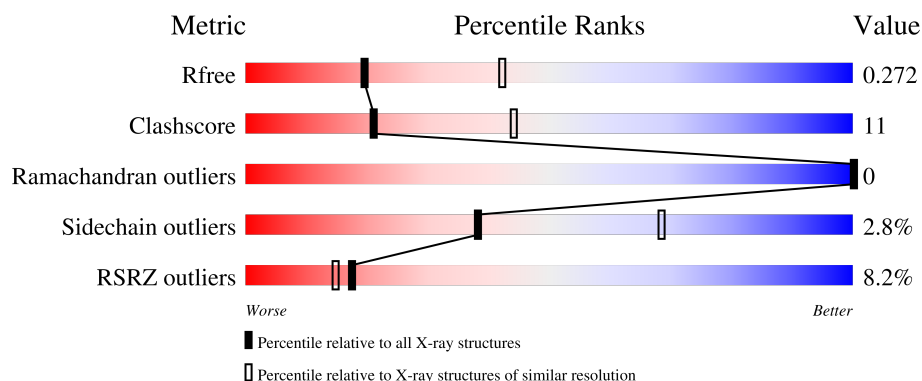
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	1191	 8% 69% 24% 7%
2	P	11	 73% 27%
3	T	16	 69% 25% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9324 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 epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1110	Total	C	N	O	S	0	0	0
			8764	5613	1456	1650	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P21951
A	-3	GLY	-	expression tag	UNP P21951
A	-2	ASP	-	expression tag	UNP P21951
A	-1	PRO	-	expression tag	UNP P21951
A	0	HIS	-	expression tag	UNP P21951
A	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	UNP P21951
A	828	VAL	ASN	engineered mutation	UNP P21951

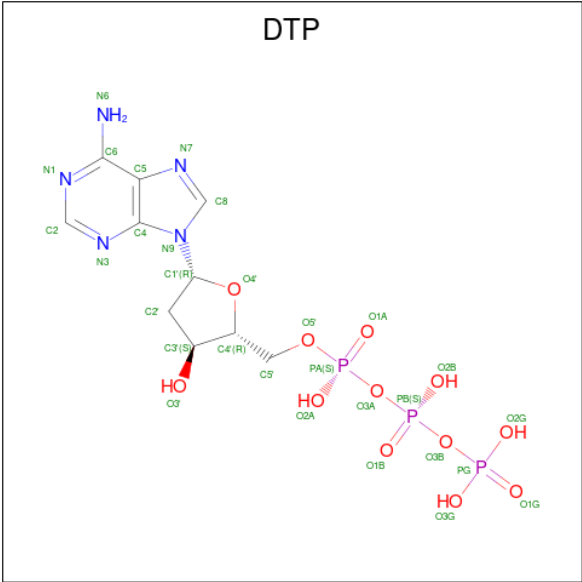
- Molecule 2 is a DNA chain called Primer DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			221	106	38	66	11			

- Molecule 3 is a DNA chain called Template DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			308	147	54	92	15			

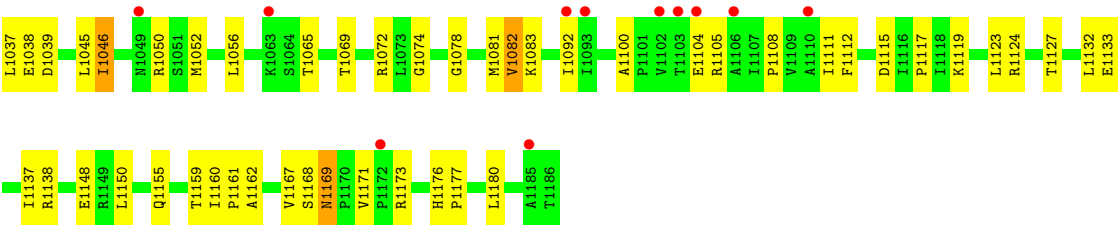
- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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



• Molecule 2: Primer DNA sequence



• Molecule 3: Template DNA sequence



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.99Å 71.03Å 155.25Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	65.49 – 2.70 65.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (65.49-2.70) 98.4 (65.49-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.236 , 0.273 0.239 , 0.272	Depositor DCC
R_{free} test set	2179 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9324	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/8965	0.51	7/12153 (0.1%)
2	P	0.53	0/226	0.85	0/346
3	T	0.28	0/344	0.54	0/529
All	All	0.28	0/9535	0.52	7/13028 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1083	LYS	N-CA-C	8.47	120.51	111.28
1	A	329	SER	N-CA-C	7.53	120.58	111.40
1	A	1082	VAL	N-CA-C	7.06	118.19	111.91
1	A	1169	ASN	N-CA-C	-6.33	100.72	109.71
1	A	330	GLU	N-CA-C	-5.93	100.33	109.76
1	A	327	ILE	N-CA-C	-5.23	107.72	112.12
1	A	329	SER	CB-CA-C	-5.12	102.19	110.79

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	A	8764	0	8406	196	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	221	0	125	2	0
3	T	308	0	171	3	0
4	A	30	0	12	1	0
5	A	1	0	0	0	0
All	All	9324	0	8714	198	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 11.

All (198) 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:310:MET:HG2	1:A:328:ILE:HD11	1.43	1.00
1:A:677:CYS:O	1:A:763:CYS:HA	1.62	0.97
1:A:310:MET:CG	1:A:328:ILE:HD11	1.97	0.94
1:A:310:MET:SD	1:A:328:ILE:HD11	2.16	0.85
1:A:1115:ASP:HB3	1:A:1117:PRO:HD2	1.68	0.73
1:A:310:MET:SD	1:A:328:ILE:CD1	2.77	0.73
1:A:454:LEU:HD12	1:A:459:MET:HG3	1.71	0.73
1:A:213:ASN:ND2	1:A:237:HIS:HA	2.04	0.72
1:A:548:LEU:HD23	1:A:689:PHE:HB3	1.72	0.72
1:A:310:MET:HE1	1:A:471:SER:HA	1.71	0.70
1:A:586:GLN:HE21	1:A:587:GLU:HG3	1.57	0.70
1:A:213:ASN:HD22	1:A:237:HIS:HA	1.58	0.68
1:A:1177:PRO:HD2	1:A:1180:LEU:HD23	1.75	0.67
1:A:836:ARG:HB2	3:T:5:DT:H4'	1.77	0.67
1:A:1112:PHE:HE1	1:A:1123:LEU:HD21	1.60	0.67
1:A:653:ARG:NH2	1:A:766:GLU:O	2.28	0.66
1:A:44:ASP:OD2	1:A:54:ARG:NH1	2.29	0.66
1:A:792:LYS:HA	1:A:813:ILE:HD11	1.77	0.65
1:A:50:MET:HE1	1:A:367:ARG:HA	1.78	0.65
1:A:296:PRO:HB2	1:A:299:LYS:HB2	1.79	0.65
1:A:573:GLU:OE2	1:A:573:GLU:N	2.23	0.64
1:A:992:LEU:HD22	1:A:994:LEU:HB3	1.79	0.64
1:A:905:TYR:O	1:A:909:MET:HG2	1.98	0.64
1:A:397:ASP:HB3	1:A:400:ASP:HB2	1.79	0.64
1:A:141:ILE:HD11	1:A:191:LEU:HD11	1.80	0.63
1:A:440:LYS:HE2	1:A:444:GLN:HE22	1.63	0.63
1:A:159:TYR:HE1	1:A:209:ILE:HD11	1.64	0.63
1:A:64:PHE:CD1	1:A:270:GLN:HG2	2.33	0.62
1:A:337:TYR:HE2	1:A:452:ILE:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HB	1:A:394:HIS:HD2	1.66	0.60
1:A:1112:PHE:CD2	1:A:1137:ILE:HG13	2.36	0.60
1:A:989:ARG:HH21	2:P:8:DG:P	2.23	0.60
1:A:50:MET:HE3	1:A:50:MET:HA	1.83	0.59
1:A:164:LEU:HD11	1:A:191:LEU:HD22	1.84	0.59
1:A:700:ILE:HG13	1:A:739:LEU:HD13	1.83	0.59
1:A:1045:LEU:O	1:A:1045:LEU:HD23	2.01	0.59
1:A:918:PHE:O	1:A:940:ASN:ND2	2.35	0.59
1:A:337:TYR:CD1	1:A:339:PRO:HD3	2.38	0.59
3:T:11:DC:H2"	3:T:12:DG:C8	2.38	0.59
1:A:778:ARG:NH1	1:A:779:ASP:OD1	2.35	0.58
1:A:960:GLU:N	1:A:960:GLU:OE2	2.35	0.58
1:A:159:TYR:CE1	1:A:209:ILE:HD11	2.38	0.57
1:A:352:GLU:CD	1:A:361:ARG:HE	2.12	0.57
1:A:1072:ARG:NH2	1:A:1104:GLU:O	2.38	0.57
1:A:1167:VAL:HG12	1:A:1168:SER:O	2.05	0.57
1:A:261:VAL:HG11	1:A:504:PRO:HD3	1.88	0.56
1:A:586:GLN:NE2	1:A:587:GLU:HG3	2.20	0.56
1:A:552:THR:OG1	1:A:553:TYR:N	2.37	0.56
1:A:310:MET:HG2	1:A:328:ILE:CD1	2.28	0.56
1:A:33:SER:O	1:A:37:LEU:HD12	2.07	0.55
1:A:596:VAL:HG12	1:A:602:SER:HB2	1.88	0.55
1:A:496:LEU:HG	1:A:500:ILE:HD12	1.89	0.55
1:A:924:GLN:CG	1:A:936:THR:HG22	2.36	0.55
1:A:994:LEU:HD11	1:A:1150:LEU:HD22	1.88	0.55
1:A:510:LYS:HD2	1:A:514:THR:HG21	1.89	0.54
1:A:728:TYR:O	1:A:732:VAL:HG23	2.06	0.54
1:A:1028:ASP:OD1	1:A:1173:ARG:NH1	2.36	0.54
1:A:845:GLU:O	1:A:849:ILE:HG13	2.07	0.54
1:A:924:GLN:HE21	1:A:936:THR:CG2	2.21	0.53
1:A:810:LYS:O	1:A:814:VAL:HG23	2.09	0.53
1:A:1133:GLU:N	1:A:1133:GLU:OE1	2.41	0.53
1:A:354:ASP:N	1:A:354:ASP:OD1	2.39	0.53
1:A:323:THR:HB	1:A:328:ILE:HD12	1.91	0.52
1:A:393:ILE:HG23	1:A:394:HIS:ND1	2.24	0.52
1:A:592:LEU:HB3	1:A:610:PHE:CE1	2.44	0.52
1:A:503:ASN:OD1	1:A:506:GLU:HG3	2.08	0.52
1:A:541:ARG:HG3	1:A:548:LEU:HD12	1.90	0.52
1:A:337:TYR:CE2	1:A:452:ILE:HD12	2.44	0.52
1:A:760:ALA:HB3	1:A:849:ILE:HD11	1.91	0.52
1:A:1056:LEU:HB2	1:A:1082:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:ASP:O	1:A:1011:THR:OG1	2.25	0.52
1:A:679:ARG:HB3	1:A:762:VAL:HG13	1.91	0.52
1:A:322:ILE:HG23	1:A:350:PHE:HB2	1.92	0.52
1:A:1002:ILE:HD12	1:A:1003:PHE:N	2.25	0.52
1:A:337:TYR:HD1	1:A:339:PRO:HD3	1.73	0.51
1:A:1082:VAL:HG12	1:A:1082:VAL:O	2.10	0.51
2:P:1:DT:H2"	2:P:2:DA:C8	2.45	0.51
1:A:644:MET:SD	1:A:877:ASP:HB3	2.50	0.51
1:A:261:VAL:HB	1:A:497:CYS:HB3	1.92	0.51
1:A:608:THR:OG1	1:A:609:ASN:N	2.43	0.51
1:A:1031:ASP:OD2	1:A:1173:ARG:NH2	2.43	0.51
1:A:1119:LYS:HG2	1:A:1123:LEU:HD13	1.93	0.51
1:A:804:HIS:O	1:A:808:GLU:HG2	2.11	0.50
1:A:653:ARG:HG3	1:A:923:TYR:CE2	2.46	0.50
1:A:314:MET:HE1	1:A:483:TYR:CE2	2.46	0.50
1:A:201:GLU:HA	1:A:204:LYS:HD2	1.93	0.50
1:A:651:THR:HG23	1:A:940:ASN:HA	1.93	0.49
1:A:321:LEU:HB3	1:A:349:ILE:HG13	1.95	0.49
1:A:1100:ALA:O	1:A:1105:ARG:NH1	2.42	0.49
1:A:658:SER:HB3	1:A:762:VAL:HG23	1.95	0.49
1:A:209:ILE:O	1:A:212:ASP:N	2.45	0.49
1:A:33:SER:C	1:A:37:LEU:HD12	2.38	0.48
1:A:1029:VAL:HA	1:A:1036:MET:HE3	1.94	0.48
1:A:383:ASP:O	1:A:387:ILE:HG13	2.13	0.48
1:A:207:ARG:O	1:A:211:GLN:HG3	2.13	0.48
1:A:594:PHE:CE2	1:A:915:HIS:HD2	2.32	0.48
1:A:951:LYS:HD3	1:A:1007:LEU:HD23	1.95	0.48
1:A:1038:GLU:H	1:A:1038:GLU:CD	2.22	0.48
1:A:686:ARG:HG3	1:A:755:ILE:CD1	2.44	0.48
1:A:691:PRO:HD2	1:A:743:SER:HB3	1.94	0.48
1:A:261:VAL:HG21	1:A:503:ASN:HA	1.96	0.47
1:A:379:GLY:HA2	1:A:383:ASP:HB2	1.96	0.47
1:A:572:ASN:HD22	1:A:870:ARG:HH12	1.63	0.47
1:A:636:ILE:HG12	1:A:882:ILE:HG22	1.96	0.47
1:A:655:GLN:HG3	1:A:658:SER:HB2	1.97	0.47
1:A:1160:ILE:HB	1:A:1161:PRO:HD3	1.96	0.47
1:A:914:VAL:O	1:A:918:PHE:N	2.43	0.47
1:A:1065:THR:O	1:A:1069:THR:OG1	2.24	0.47
1:A:645:TYR:CG	4:A:1301:DTP:H2'1	2.50	0.47
1:A:310:MET:SD	1:A:328:ILE:HD13	2.54	0.46
1:A:594:PHE:CE2	1:A:915:HIS:CD2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TYR:CE1	1:A:1162:ALA:HB2	2.50	0.46
1:A:333:GLU:C	1:A:349:ILE:HD13	2.40	0.46
1:A:972:PHE:CD2	1:A:1007:LEU:HD11	2.50	0.46
1:A:287:MET:HB2	1:A:315:ILE:HG12	1.98	0.46
1:A:998:PHE:CE1	1:A:1002:ILE:HG21	2.50	0.46
1:A:485:TYR:CZ	1:A:490:HIS:HB2	2.50	0.46
1:A:438:GLY:O	1:A:442:VAL:HG13	2.16	0.46
1:A:1013:GLU:HG3	1:A:1167:VAL:HG22	1.98	0.46
1:A:454:LEU:HD12	1:A:459:MET:CG	2.43	0.46
1:A:279:ILE:HD12	1:A:280:ALA:N	2.30	0.45
1:A:1123:LEU:O	1:A:1127:THR:OG1	2.24	0.45
1:A:845:GLU:OE1	1:A:845:GLU:N	2.32	0.45
1:A:1108:PRO:O	1:A:1111:ILE:HG22	2.16	0.45
1:A:295:LYS:NZ	1:A:456:PRO:O	2.49	0.45
1:A:308:ILE:CD1	1:A:390:ARG:HG3	2.47	0.45
1:A:322:ILE:HG22	1:A:358:LEU:HD12	1.97	0.45
1:A:872:LEU:HD21	1:A:882:ILE:HG12	1.99	0.45
1:A:78:TRP:CE3	1:A:80:THR:HG22	2.51	0.45
1:A:339:PRO:HG2	1:A:343:TYR:HB2	1.98	0.45
1:A:390:ARG:HA	1:A:393:ILE:HG22	1.98	0.45
1:A:1112:PHE:CE1	1:A:1123:LEU:HD21	2.46	0.45
1:A:244:GLU:OE1	1:A:252:ARG:NH2	2.50	0.44
1:A:924:GLN:HG3	1:A:936:THR:HG22	1.97	0.44
1:A:456:PRO:HA	1:A:459:MET:HE2	1.99	0.44
1:A:967:LYS:HD2	3:T:9:DC:H4'	2.00	0.44
1:A:295:LYS:HZ1	1:A:456:PRO:C	2.25	0.44
1:A:312:SER:HB3	1:A:474:SER:OG	2.17	0.44
1:A:1039:ASP:CG	1:A:1138:ARG:HH12	2.25	0.44
1:A:1046:ILE:HG22	1:A:1092:ILE:HD11	2.00	0.44
1:A:1169:ASN:HB2	1:A:1176:HIS:CE1	2.52	0.44
1:A:860:MET:HE1	1:A:914:VAL:HG22	1.99	0.44
1:A:964:GLY:O	1:A:965:ILE:HD13	2.18	0.43
1:A:267:VAL:HG13	1:A:272:PHE:CE1	2.53	0.43
1:A:440:LYS:HE2	1:A:444:GLN:NE2	2.30	0.43
1:A:86:LEU:HD12	1:A:115:SER:HA	2.00	0.43
1:A:609:ASN:HB2	1:A:612:GLU:HB3	2.00	0.43
1:A:1124:ARG:HH21	1:A:1132:LEU:C	2.26	0.43
1:A:207:ARG:N	1:A:208:PRO:HD2	2.34	0.43
1:A:857:ILE:HG13	1:A:918:PHE:CD2	2.53	0.43
1:A:164:LEU:HD21	1:A:167:LEU:HB3	2.01	0.43
1:A:679:ARG:HD2	1:A:922:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:PRO:HG2	1:A:749:ARG:HG3	2.00	0.43
1:A:452:ILE:HG22	1:A:473:TYR:HD1	1.83	0.43
1:A:736:LYS:O	1:A:740:THR:HG23	2.18	0.43
1:A:78:TRP:CE3	1:A:282:ALA:HB3	2.54	0.43
1:A:655:GLN:OE1	1:A:771:VAL:HG12	2.18	0.43
1:A:993:GLN:HE21	1:A:997:ASN:CG	2.27	0.43
1:A:639:VAL:HG12	1:A:946:VAL:HG23	2.01	0.43
1:A:953:MET:HG3	1:A:971:VAL:HG22	2.01	0.43
1:A:180:HIS:NE2	1:A:766:GLU:OE1	2.40	0.42
1:A:649:MET:HA	1:A:654:LEU:HB2	2.00	0.42
1:A:1008:GLU:O	1:A:1015:CYS:HA	2.19	0.42
1:A:592:LEU:HD23	1:A:592:LEU:HA	1.74	0.42
1:A:1029:VAL:HG11	1:A:1037:LEU:HD11	2.01	0.42
1:A:645:TYR:HE2	1:A:851:CYS:HG	1.64	0.42
1:A:157:LYS:HE3	1:A:167:LEU:HD11	2.01	0.42
1:A:1081:MET:HE3	1:A:1081:MET:HB3	1.86	0.42
1:A:1155:GLN:HA	1:A:1159:THR:OG1	2.19	0.42
1:A:683:TRP:HB3	1:A:849:ILE:HG12	2.01	0.42
1:A:887:PHE:CG	1:A:888:PRO:HD2	2.55	0.42
1:A:252:ARG:HA	1:A:252:ARG:HD3	1.87	0.42
1:A:287:MET:HE1	1:A:366:ILE:HD13	2.02	0.42
1:A:1171:VAL:O	1:A:1171:VAL:HG12	2.18	0.42
1:A:114:ILE:HD11	1:A:134:VAL:HG11	2.01	0.41
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.84	0.41
1:A:325:ARG:HE	1:A:325:ARG:HB3	1.73	0.41
1:A:781:ARG:NH2	1:A:820:GLN:OE1	2.53	0.41
1:A:338:THR:HG23	1:A:344:PRO:HA	2.02	0.41
1:A:76:VAL:HA	1:A:266:LYS:HA	2.03	0.41
1:A:466:LYS:HB3	1:A:466:LYS:HZ3	1.86	0.41
1:A:831:TYR:O	1:A:834:VAL:HG22	2.20	0.41
1:A:920:ASN:O	1:A:938:SER:HA	2.20	0.41
1:A:222:ILE:H	1:A:222:ILE:HG13	1.70	0.41
1:A:324:ASN:HD22	1:A:327:ILE:HG13	1.84	0.41
1:A:572:ASN:OD1	1:A:634:PRO:HG3	2.21	0.41
1:A:683:TRP:CZ2	1:A:758:ARG:HD2	2.56	0.41
1:A:309:MET:SD	1:A:470:LEU:HD21	2.60	0.41
1:A:426:VAL:HA	1:A:430:SER:HB3	2.02	0.41
1:A:573:GLU:HB3	1:A:631:ASN:OD1	2.20	0.41
1:A:1074:GLY:O	1:A:1078:GLY:N	2.52	0.41
1:A:78:TRP:HB2	1:A:264:TRP:CH2	2.55	0.41
1:A:485:TYR:CE2	1:A:490:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HD23	1:A:1035:LEU:HA	1.92	0.40
1:A:649:MET:HE3	1:A:774:VAL:HG11	2.03	0.40
1:A:695:ASP:OD1	1:A:696:GLU:N	2.54	0.40
1:A:567:ARG:HB2	1:A:570:LEU:HG	2.03	0.40
1:A:968:ARG:HA	1:A:982:LYS:O	2.20	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	1100/1191 (92%)	1042 (95%)	58 (5%)	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	
1	A	926/1065 (87%)	900 (97%)	26 (3%)	38	68

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU

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Mol	Chain	Res	Type
1	A	88	SER
1	A	150	ASN
1	A	164	LEU
1	A	184	LEU
1	A	279	ILE
1	A	327	ILE
1	A	364	GLU
1	A	372	THR
1	A	452	ILE
1	A	544	ASP
1	A	581	ILE
1	A	676	THR
1	A	757	GLU
1	A	762	VAL
1	A	785	LYS
1	A	818	SER
1	A	831	TYR
1	A	839	SER
1	A	897	ASN
1	A	935	GLU
1	A	968	ARG
1	A	1046	ILE
1	A	1050	ARG
1	A	1052	MET
1	A	1148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	HIS
1	A	360	GLN
1	A	444	GLN
1	A	586	GLN
1	A	924	GLN
1	A	993	GLN
1	A	1062	GLN
1	A	1176	HIS

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	$\# Z > 2$
2	DOC	P	11	3,2	16,19,20	0.38	0	20,26,29	0.34	0

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	DOC	P	11	3,2	-	2/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	11	DOC	C3'-C4'-C5'-O5'
2	P	11	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	DTP	A	1301	5	31,32,32	0.58	0	46,50,50	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	1301	5	-	7/22/34/34	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

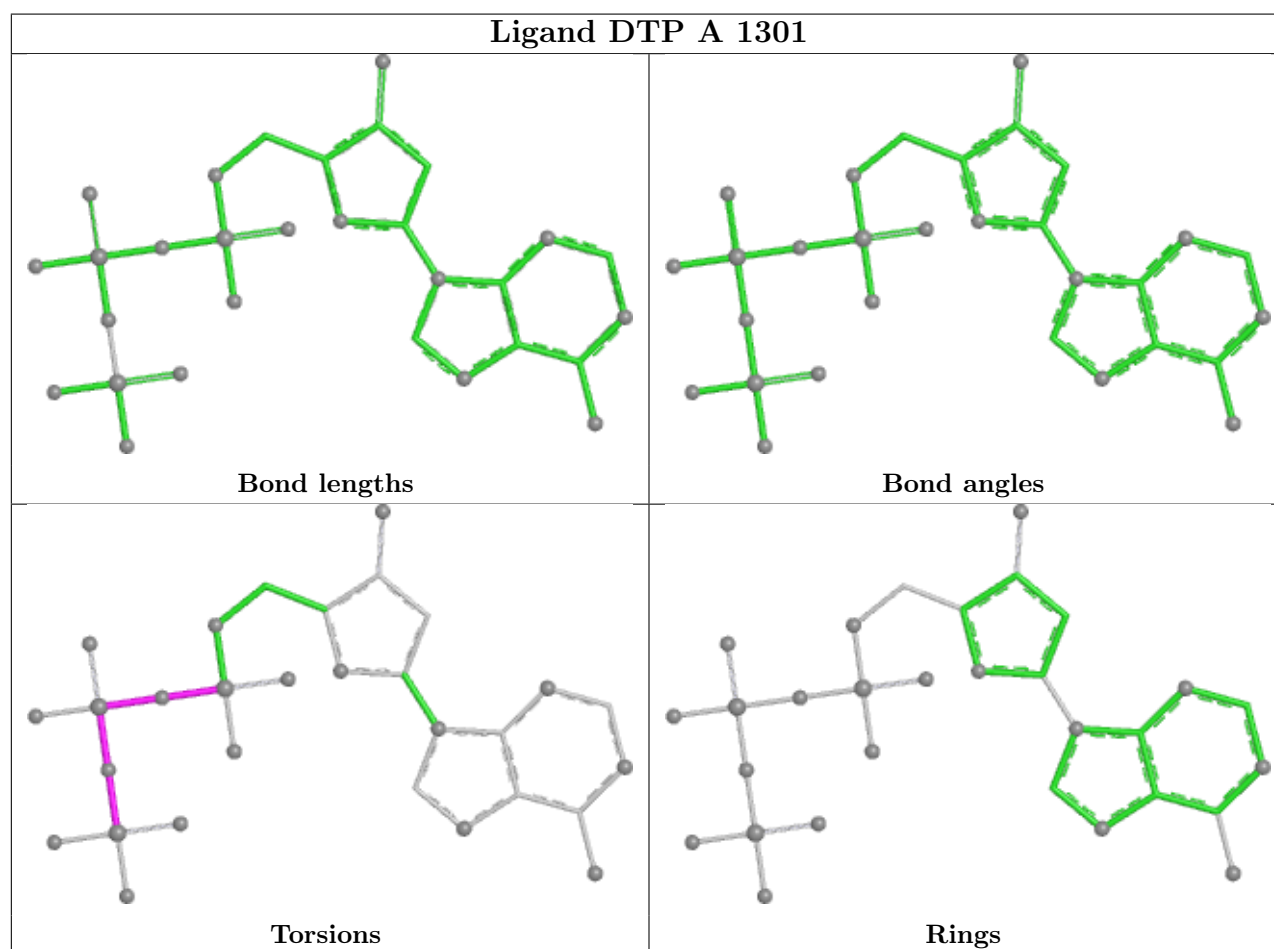
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3B-PG-O3G
4	A	1301	DTP	PB-O3A-PA-O1A
4	A	1301	DTP	PB-O3B-PG-O1G
4	A	1301	DTP	PA-O3A-PB-O1B
4	A	1301	DTP	PB-O3A-PA-O2A
4	A	1301	DTP	PA-O3A-PB-O2B
4	A	1301	DTP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	1110/1191 (93%)	0.66	93 (8%) 17 14	39, 84, 121, 162	0
2	P	10/11 (90%)	0.05	0 100 100	51, 64, 104, 122	0
3	T	15/16 (93%)	-0.07	0 100 100	46, 66, 108, 120	0
All	All	1135/1218 (93%)	0.64	93 (8%) 17 15	39, 83, 121, 162	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	VAL	6.5
1	A	665	CYS	6.1
1	A	677	CYS	5.8
1	A	225	VAL	4.7
1	A	220	ARG	4.4
1	A	750	VAL	4.4
1	A	298	LEU	4.3
1	A	967	LYS	4.1
1	A	1104	GLU	4.1
1	A	799	ASP	4.1
1	A	223	TYR	4.0
1	A	763	CYS	3.8
1	A	669	ASP	3.8
1	A	700	ILE	3.7
1	A	697	TYR	3.4
1	A	895	LEU	3.3
1	A	707	GLU	3.2
1	A	802	ASP	3.2
1	A	744	ARG	3.1
1	A	708	THR	3.1
1	A	696	GLU	3.0
1	A	1093	ILE	3.0
1	A	887	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	661	ALA	2.9
1	A	219	GLN	2.9
1	A	222	ILE	2.9
1	A	919	THR	2.9
1	A	645	TYR	2.8
1	A	742	TYR	2.8
1	A	592	LEU	2.7
1	A	182	LEU	2.7
1	A	1035	LEU	2.7
1	A	545	GLY	2.7
1	A	899	LYS	2.7
1	A	900	LYS	2.7
1	A	1185	ALA	2.7
1	A	705	GLN	2.6
1	A	549	GLU	2.6
1	A	1021	SER	2.6
1	A	876	THR	2.6
1	A	704	LEU	2.6
1	A	1029	VAL	2.6
1	A	726	LEU	2.6
1	A	747	TYR	2.6
1	A	874	LEU	2.5
1	A	745	LYS	2.5
1	A	831	TYR	2.5
1	A	31	ALA	2.5
1	A	215	ASN	2.5
1	A	1063	LYS	2.5
1	A	555	GLY	2.5
1	A	1102	VAL	2.5
1	A	1106	ALA	2.5
1	A	706	ASN	2.5
1	A	1172	PRO	2.5
1	A	692	SER	2.5
1	A	690	PHE	2.5
1	A	272	PHE	2.4
1	A	1092	ILE	2.4
1	A	670	PHE	2.4
1	A	1110	ALA	2.4
1	A	328	ILE	2.3
1	A	317	GLY	2.3
1	A	169	ILE	2.3
1	A	1103	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	216	ASN	2.3
1	A	691	PRO	2.3
1	A	756	VAL	2.3
1	A	371	PRO	2.3
1	A	62	GLY	2.2
1	A	639	VAL	2.2
1	A	279	ILE	2.2
1	A	694	MET	2.2
1	A	537	ASP	2.2
1	A	746	VAL	2.2
1	A	617	ILE	2.2
1	A	962	GLY	2.2
1	A	1034	GLY	2.2
1	A	287	MET	2.2
1	A	626	GLU	2.1
1	A	644	MET	2.1
1	A	901	LEU	2.1
1	A	305	VAL	2.1
1	A	596	VAL	2.1
1	A	698	ASN	2.1
1	A	323	THR	2.1
1	A	699	MET	2.1
1	A	891	TYR	2.1
1	A	1049	ASN	2.1
1	A	880	TRP	2.0
1	A	800	PRO	2.0
1	A	539	ILE	2.0
1	A	630	ARG	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
2	DOC	P	11	18/19	0.94	0.11	28,48,62,69	0

6.3 Carbohydrates [i](#)

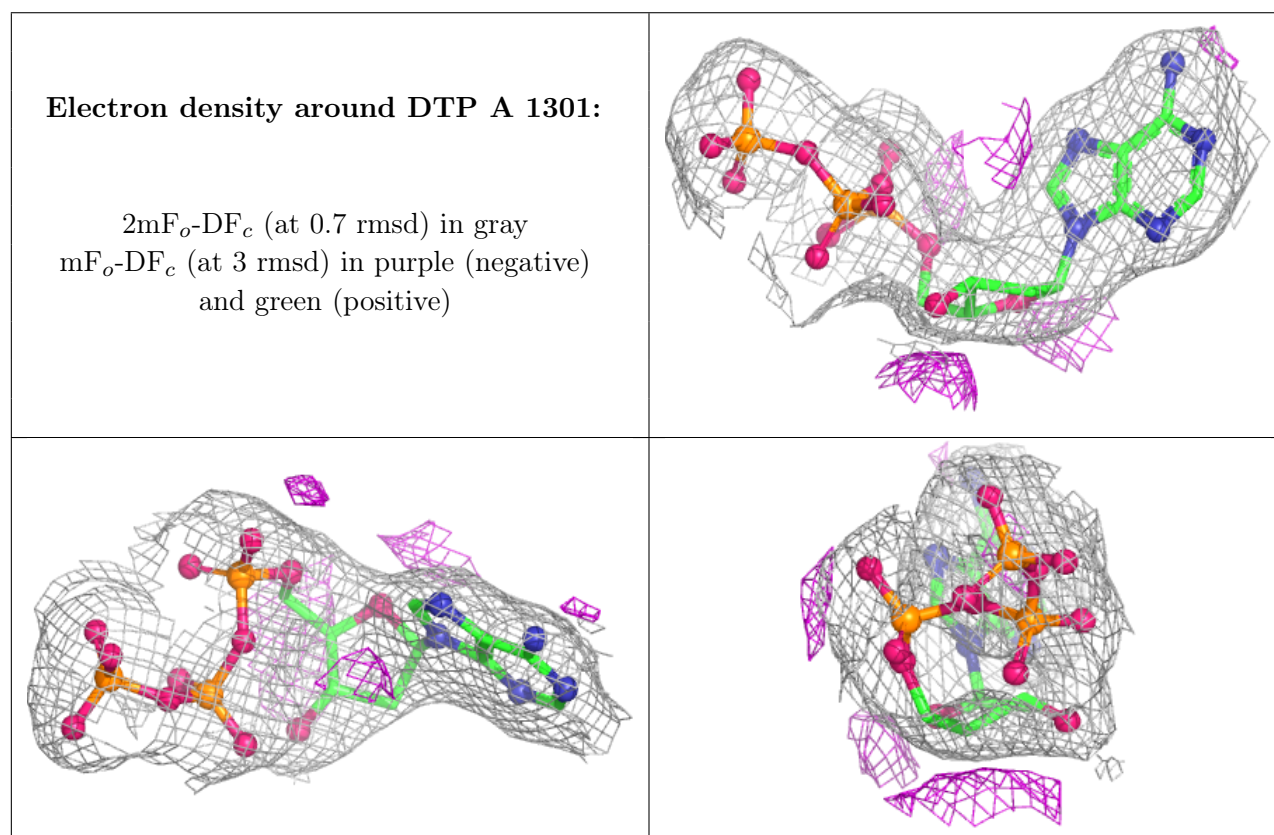
There are no oligosaccharides in this entry.

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	DTP	A	1301	30/30	0.97	0.07	28,45,57,63	0
5	CA	A	1302	1/1	0.99	0.04	65,65,65,65	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.