



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:14 PM UTC

PDB ID : 7R3X / pdb_00007r3x
Title : The crystal structure of the L439V variant of Pol2CORE in complex with DNA and an incoming nucleotide
Authors : Barbari, S.R.; Beach, A.K.; Markgren, J.G.; Parkash, V.; Johansson, E.; Shcherbakova, P.V.
Deposited on : 2022-02-08
Resolution : 2.46 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

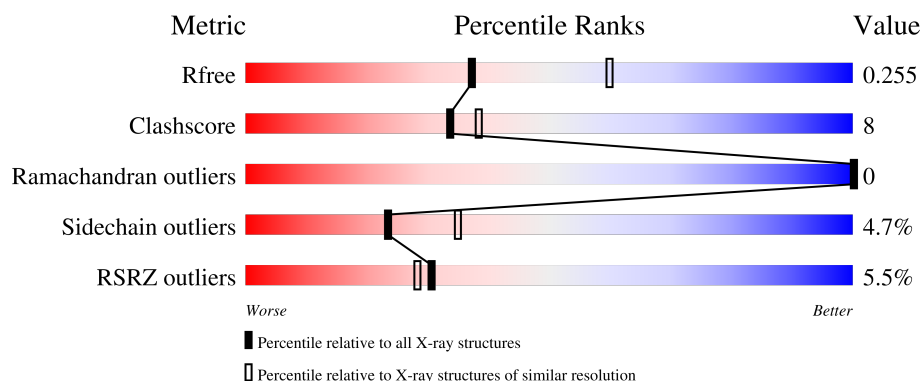
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	1185	5% 74% 19% • 5%
2	P	11	9% 45% 55%
3	T	16	38% 50% 6% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	1304	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9697 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	1122	Total	C	N	O	S	0	0	0
			9036	5789	1509	1696	42			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	439	VAL	LEU	engineered mutation	UNP P21951

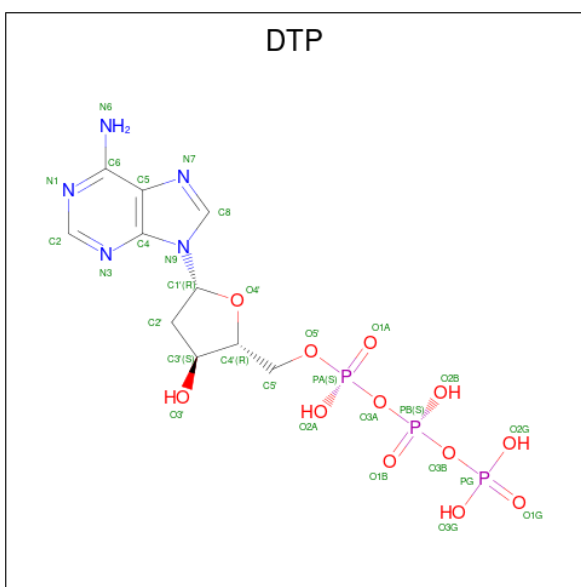
- Molecule 2 is a DNA chain called DNA Primer.

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 DNA Template.

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: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

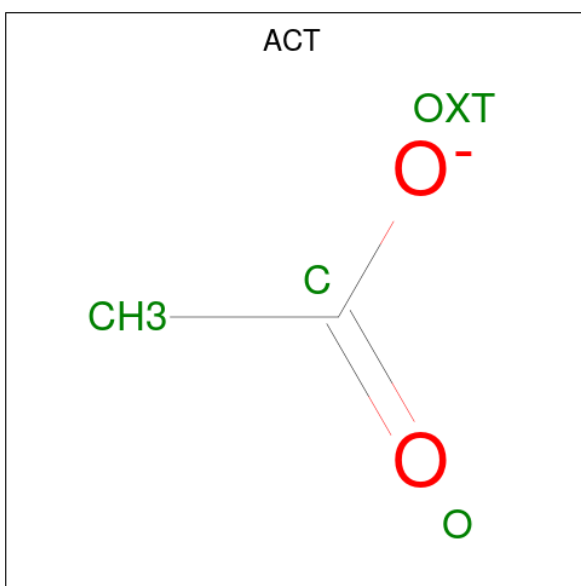


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

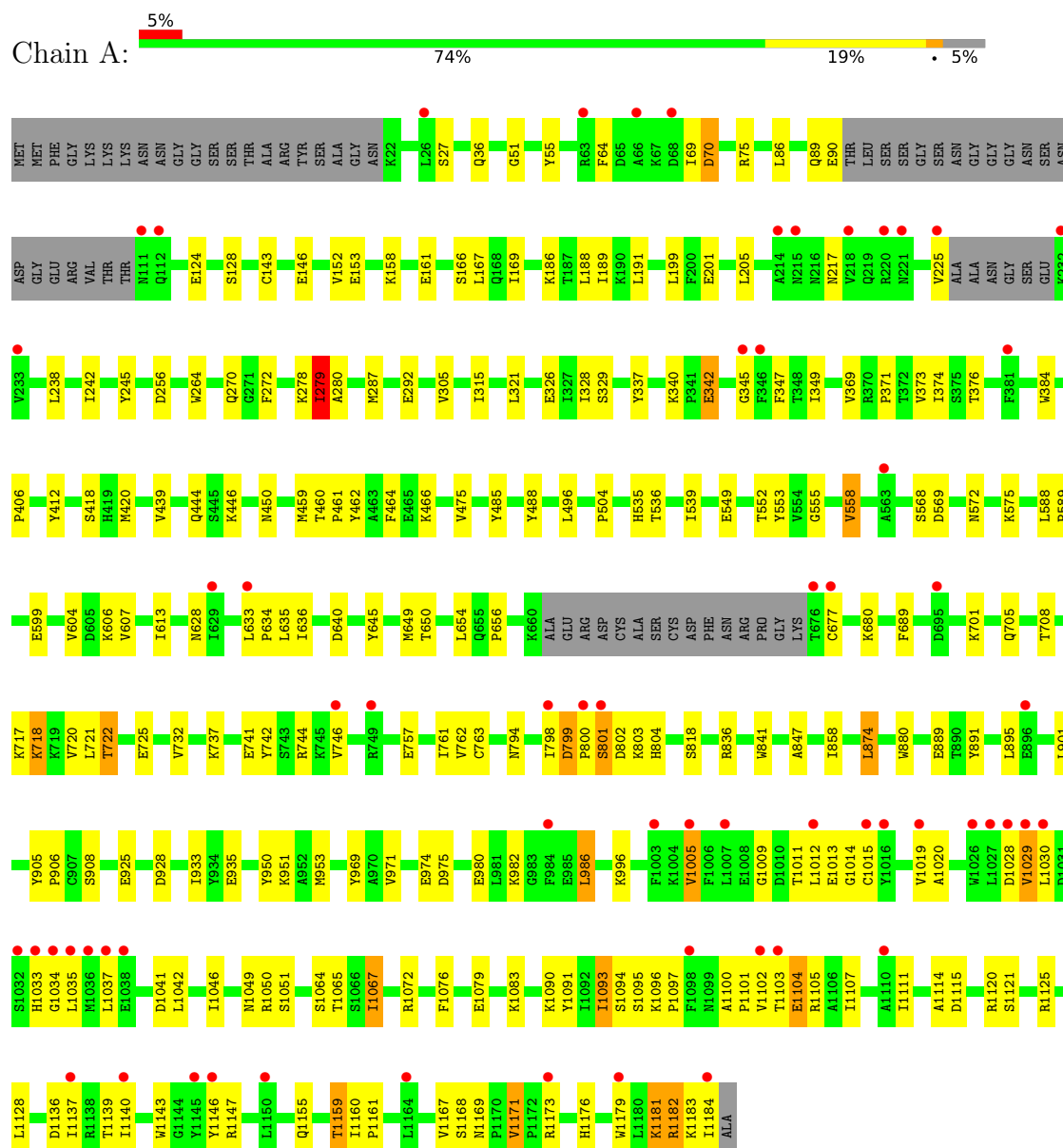
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total	O	0	0
			87	87		
7	P	1	Total	O	0	0
			1	1		
7	T	8	Total	O	0	0
			8	8		

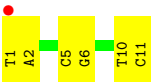
3 Residue-property plots [i](#)

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.

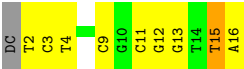
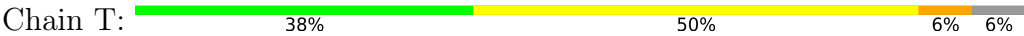
- Molecule 1: DNA polymerase epsilon catalytic subunit A



- Molecule 2: DNA Primer



● Molecule 3: DNA Template



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.50Å 70.69Å 111.64Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	45.78 – 2.46 45.78 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.78-2.46) 99.8 (45.78-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.256 0.213 , 0.255	Depositor DCC
R_{free} test set	3070 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9697	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: CA, DTP, DOC, ACT

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	1.10	7/9243 (0.1%)	1.40	25/12511 (0.2%)
2	P	0.82	0/226	1.20	0/346
3	T	0.80	0/344	1.08	2/529 (0.4%)
All	All	1.08	7/9813 (0.1%)	1.38	27/13386 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	LYS	C-O	6.66	1.31	1.24
1	A	504	PRO	C-O	-6.15	1.16	1.24
1	A	376	THR	C-O	5.84	1.31	1.23
1	A	279	ILE	C-O	5.54	1.30	1.24
1	A	406	PRO	C-O	-5.35	1.18	1.23
1	A	535	HIS	CE1-NE2	5.08	1.37	1.32
1	A	256	ASP	C-O	-5.06	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1029	VAL	N-CA-C	-11.72	102.41	111.90
1	A	1115	ASP	CA-CB-CG	8.73	121.33	112.60
1	A	1104	GLU	N-CA-C	-7.78	100.84	110.41
1	A	536	THR	CA-CB-OG1	-6.94	99.19	109.60
3	T	2	DT	P-O3'-C3'	-6.28	110.78	120.20
1	A	555	GLY	CA-C-N	6.06	125.86	120.10
1	A	555	GLY	C-N-CA	6.06	125.86	120.10
1	A	1143	TRP	CA-C-N	5.87	126.49	119.98
1	A	1143	TRP	C-N-CA	5.87	126.49	119.98
1	A	1009	GLY	CA-C-O	-5.84	118.10	122.37
1	A	326	GLU	CB-CG-CD	5.83	122.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	974	GLU	CA-C-N	5.58	128.53	120.38
1	A	974	GLU	C-N-CA	5.58	128.53	120.38
3	T	15	DT	P-O3'-C3'	-5.35	112.17	120.20
1	A	549	GLU	N-CA-C	-5.34	106.89	113.41
1	A	935	GLU	CB-CG-CD	5.24	121.51	112.60
1	A	718	LYS	CA-C-O	-5.20	115.55	120.90
1	A	146	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	1013	GLU	CA-C-N	5.14	125.66	120.00
1	A	1013	GLU	C-N-CA	5.14	125.66	120.00
1	A	1033	HIS	N-CA-C	-5.13	104.56	111.54
1	A	1034	GLY	CA-C-O	-5.09	116.41	120.79
1	A	975	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	1114	ALA	CA-C-O	-5.07	115.95	121.89
1	A	328	ILE	CA-C-N	5.04	127.54	120.28
1	A	328	ILE	C-N-CA	5.04	127.54	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9036	0	8845	138	0
2	P	221	0	125	3	0
3	T	308	0	171	7	0
4	A	30	0	12	2	0
5	A	2	0	0	0	0
6	A	4	0	3	3	0
7	A	87	0	0	0	0
7	P	1	0	0	0	0
7	T	8	0	0	0	0
All	All	9697	0	9156	144	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 8.

All (144) 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:345:GLY:O	1:A:347:PHE:CD1	2.33	0.80
1:A:1101:PRO:HB2	1:A:1103:THR:HG22	1.63	0.79
1:A:345:GLY:O	1:A:347:PHE:HD1	1.68	0.74
1:A:1103:THR:HG23	1:A:1104:GLU:N	2.01	0.74
2:P:10:DT:H2''	2:P:11:DOC:H5'	1.73	0.71
1:A:802:ASP:HB3	1:A:804:HIS:CE1	2.27	0.69
1:A:1028:ASP:CG	1:A:1173:ARG:HH22	2.02	0.67
1:A:1103:THR:HG23	1:A:1104:GLU:H	1.58	0.67
3:T:15:DT:H2''	3:T:16:DA:C8	2.29	0.66
1:A:1011:THR:HG23	1:A:1014:GLY:H	1.62	0.65
1:A:1167:VAL:HG12	1:A:1168:SER:O	1.96	0.65
1:A:1121:SER:O	1:A:1125:ARG:HG3	1.96	0.64
1:A:1103:THR:CG2	1:A:1104:GLU:H	2.11	0.63
1:A:1104:GLU:O	1:A:1105:ARG:HB2	1.97	0.63
1:A:1102:VAL:HG11	3:T:13:DG:H5'	1.81	0.63
1:A:708:THR:HB	1:A:720:VAL:HG13	1.81	0.62
1:A:1103:THR:CG2	1:A:1104:GLU:N	2.64	0.61
1:A:439:VAL:CG2	6:A:1304:ACT:H2	2.31	0.61
1:A:1035:LEU:HD12	1:A:1042:LEU:HD23	1.83	0.61
1:A:1030:LEU:HD21	1:A:1147:ARG:HA	1.83	0.61
1:A:1094:SER:O	1:A:1105:ARG:HD2	2.01	0.61
1:A:439:VAL:HG21	6:A:1304:ACT:H2	1.83	0.61
1:A:1046:ILE:HG23	1:A:1146:TYR:CE2	2.37	0.60
1:A:836:ARG:HH22	3:T:4:DT:H72	1.68	0.59
1:A:1102:VAL:CG1	3:T:13:DG:H5'	2.32	0.59
1:A:701:LYS:O	1:A:705:GLN:HG3	2.02	0.59
2:P:1:DT:H2''	2:P:2:DA:C8	2.37	0.59
1:A:1035:LEU:HD13	1:A:1037:LEU:HG	1.85	0.58
1:A:1155:GLN:HA	1:A:1159:THR:HB	1.84	0.58
1:A:645:TYR:CD2	4:A:1301:DTP:H2'1	2.39	0.58
1:A:152:VAL:HG23	1:A:189:ILE:HD11	1.86	0.57
1:A:124:GLU:OE2	1:A:278:LYS:HE2	2.04	0.57
1:A:89:GLN:O	1:A:90:GLU:C	2.48	0.56
1:A:794:ASN:O	1:A:798:ILE:HG12	2.07	0.55
1:A:645:TYR:CG	4:A:1301:DTP:H2'1	2.41	0.55
1:A:152:VAL:HG23	1:A:189:ILE:CD1	2.37	0.55
1:A:292:GLU:OE1	1:A:459:MET:HE1	2.07	0.55
1:A:858:ILE:HG13	1:A:874:LEU:HD11	1.89	0.55
1:A:444:GLN:NE2	1:A:450:ASN:OD1	2.40	0.55
1:A:242:ILE:HG13	1:A:245:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:ILE:H	1:A:1137:ILE:HD12	1.72	0.54
1:A:329:SER:OG	1:A:464:PHE:HA	2.08	0.53
1:A:287:MET:O	1:A:374:ILE:HA	2.08	0.53
1:A:1020:ALA:CB	1:A:1171:VAL:HG22	2.38	0.53
1:A:635:LEU:HD13	1:A:889:GLU:CD	2.33	0.52
1:A:741:GLU:HA	1:A:744:ARG:HD3	1.90	0.52
1:A:1035:LEU:HD13	1:A:1037:LEU:CD1	2.39	0.52
1:A:153:GLU:OE1	1:A:169:ILE:HD11	2.10	0.52
1:A:143:CYS:SG	1:A:152:VAL:HG21	2.49	0.52
1:A:287:MET:HG3	1:A:315:ILE:HG12	1.93	0.51
1:A:321:LEU:HB3	1:A:349:ILE:HD12	1.92	0.51
1:A:539:ILE:HG22	1:A:732:VAL:HG21	1.92	0.51
1:A:799:ASP:O	1:A:800:PRO:C	2.54	0.51
1:A:69:ILE:HG23	1:A:70:ASP:OD1	2.11	0.51
1:A:1064:SER:OG	1:A:1067:ILE:HD12	2.11	0.51
1:A:462:TYR:CZ	1:A:466:LYS:HE2	2.45	0.50
1:A:1093:ILE:HA	1:A:1105:ARG:O	2.11	0.50
1:A:1093:ILE:HD11	1:A:1146:TYR:CE1	2.46	0.50
1:A:801:SER:O	1:A:802:ASP:C	2.54	0.50
1:A:1181:LYS:HA	1:A:1184:ILE:CD1	2.42	0.50
1:A:64:PHE:HA	1:A:270:GLN:HE22	1.77	0.50
3:T:11:DC:H2"	3:T:12:DG:C8	2.47	0.49
1:A:1169:ASN:HB2	1:A:1176:HIS:NE2	2.26	0.49
1:A:677:CYS:O	1:A:763:CYS:HA	2.13	0.49
1:A:1094:SER:HB3	1:A:1105:ARG:HG2	1.95	0.49
1:A:613:ILE:HD12	1:A:891:TYR:HB3	1.95	0.49
1:A:369:VAL:HG23	1:A:371:PRO:HD3	1.96	0.48
1:A:1093:ILE:HD11	1:A:1146:TYR:CZ	2.48	0.48
1:A:722:THR:HG23	1:A:725:GLU:OE2	2.13	0.48
2:P:5:DC:H2"	2:P:6:DG:C8	2.48	0.48
1:A:345:GLY:O	1:A:347:PHE:CE1	2.67	0.48
1:A:418:SER:HB3	1:A:420:MET:HE3	1.96	0.48
1:A:1093:ILE:HD12	1:A:1093:ILE:O	2.14	0.47
1:A:568:SER:HB2	1:A:951:LYS:HA	1.95	0.47
1:A:742:TYR:CZ	1:A:746:VAL:HG21	2.49	0.47
1:A:1005:VAL:CG2	1:A:1019:VAL:HA	2.44	0.47
1:A:340:LYS:HG2	1:A:342:GLU:HG2	1.96	0.47
1:A:635:LEU:HD13	1:A:889:GLU:OE2	2.15	0.47
1:A:953:MET:HE3	1:A:971:VAL:CG2	2.44	0.47
1:A:1011:THR:HG23	1:A:1014:GLY:N	2.28	0.47
1:A:636:ILE:HD12	1:A:950:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HG13	1:A:280:ALA:H	1.80	0.46
1:A:1049:ASN:O	1:A:1050:ARG:HG3	2.16	0.46
1:A:201:GLU:O	1:A:205:LEU:HD23	2.15	0.46
1:A:1096:LYS:HA	1:A:1097:PRO:C	2.40	0.46
1:A:347:PHE:CE1	1:A:475:VAL:HG13	2.52	0.45
1:A:1035:LEU:HD13	1:A:1037:LEU:CG	2.46	0.45
1:A:199:LEU:C	1:A:199:LEU:HD23	2.41	0.45
1:A:905:TYR:N	1:A:906:PRO:HD2	2.32	0.45
3:T:3:DC:H2''	3:T:4:DT:O5'	2.16	0.45
1:A:64:PHE:HA	1:A:270:GLN:NE2	2.32	0.44
1:A:575:LYS:HB3	1:A:575:LYS:HE3	1.86	0.44
1:A:680:LYS:HG2	1:A:761:ILE:HD13	1.99	0.44
1:A:1100:ALA:O	1:A:1105:ARG:NH2	2.44	0.44
1:A:1179:TRP:HA	1:A:1182:ARG:CZ	2.47	0.44
1:A:606:LYS:O	1:A:895:LEU:HA	2.18	0.44
1:A:1011:THR:OG1	1:A:1012:LEU:N	2.50	0.44
1:A:373:VAL:HG11	1:A:485:TYR:CZ	2.52	0.44
1:A:880:TRP:CG	1:A:953:MET:HE1	2.53	0.44
1:A:446:LYS:HB3	1:A:488:TYR:CE2	2.53	0.44
1:A:1065:THR:HG21	1:A:1091:TYR:OH	2.17	0.44
1:A:152:VAL:CG1	1:A:238:LEU:HB2	2.48	0.43
1:A:1102:VAL:O	1:A:1104:GLU:O	2.36	0.43
1:A:337:TYR:O	1:A:345:GLY:HA3	2.18	0.43
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.53	0.43
1:A:158:LYS:O	1:A:161:GLU:HG3	2.18	0.43
1:A:189:ILE:HG22	1:A:191:LEU:HD12	1.99	0.43
1:A:1097:PRO:HG3	1:A:1128:LEU:HD12	2.01	0.43
1:A:552:THR:OG1	1:A:553:TYR:N	2.48	0.43
1:A:572:ASN:OD1	1:A:634:PRO:HG3	2.19	0.43
1:A:895:LEU:HD11	1:A:901:LEU:HG	2.01	0.43
1:A:656:PRO:HG2	1:A:841:TRP:HB3	2.01	0.43
1:A:558:VAL:HG13	3:T:9:DC:OP1	2.19	0.43
1:A:1136:ASP:O	1:A:1139:THR:HG22	2.19	0.42
1:A:36:GLN:HB3	1:A:86:LEU:CD1	2.49	0.42
1:A:1095:SER:N	1:A:1140:ILE:O	2.52	0.42
1:A:51:GLY:O	1:A:128:SER:OG	2.35	0.42
1:A:708:THR:HB	1:A:720:VAL:CG1	2.48	0.42
1:A:880:TRP:CD2	1:A:953:MET:HE1	2.54	0.42
1:A:460:THR:HB	1:A:461:PRO:HD3	2.02	0.42
1:A:1101:PRO:HB2	1:A:1103:THR:CG2	2.44	0.42
1:A:384:TRP:HB3	1:A:412:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:VAL:O	1:A:607:VAL:HG12	2.19	0.42
1:A:153:GLU:HG3	1:A:167:LEU:HD21	2.01	0.42
1:A:599:GLU:OE2	1:A:908:SER:OG	2.31	0.42
1:A:953:MET:HE3	1:A:971:VAL:HG22	2.01	0.41
1:A:553:TYR:CZ	1:A:847:ALA:HB1	2.55	0.41
1:A:568:SER:O	1:A:633:LEU:HD21	2.20	0.41
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.93	0.41
1:A:742:TYR:CD1	1:A:742:TYR:C	2.98	0.41
1:A:347:PHE:CZ	1:A:475:VAL:HG13	2.56	0.41
1:A:1160:ILE:N	1:A:1161:PRO:CD	2.84	0.41
1:A:55:TYR:CZ	1:A:75:ARG:HB2	2.55	0.41
1:A:654:LEU:HD23	1:A:762:VAL:HG11	2.01	0.41
1:A:588:LEU:HB3	1:A:589:PRO:HD3	2.03	0.41
1:A:986:LEU:HA	1:A:996:LYS:HG2	2.03	0.41
1:A:439:VAL:HG23	6:A:1304:ACT:H2	2.01	0.41
1:A:1181:LYS:O	1:A:1184:ILE:HG12	2.21	0.41
1:A:649:MET:HA	1:A:654:LEU:HB2	2.03	0.40
1:A:928:ASP:HB3	1:A:933:ILE:HB	2.03	0.40
1:A:272:PHE:N	1:A:272:PHE:CD1	2.88	0.40
1:A:1111:ILE:HD12	1:A:1111:ILE:HA	1.91	0.40
1:A:186:LYS:HD3	1:A:188:LEU:HD21	2.03	0.40
1:A:264:TRP:CD1	1:A:278:LYS:HB3	2.56	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	1114/1185 (94%)	1065 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	986/1063 (93%)	940 (95%)	46 (5%)	23	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	70	ASP
1	A	166	SER
1	A	225	VAL
1	A	279	ILE
1	A	305	VAL
1	A	342	GLU
1	A	558	VAL
1	A	569	ASP
1	A	628	ASN
1	A	640	ASP
1	A	650	THR
1	A	689	PHE
1	A	717	LYS
1	A	718	LYS
1	A	721	LEU
1	A	722	THR
1	A	737	LYS
1	A	757	GLU
1	A	799	ASP
1	A	801	SER
1	A	803	LYS
1	A	818	SER
1	A	874	LEU
1	A	925	GLU
1	A	980	GLU
1	A	986	LEU
1	A	1005	VAL
1	A	1015	CYS
1	A	1029	VAL

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Mol	Chain	Res	Type
1	A	1041	ASP
1	A	1051	SER
1	A	1067	ILE
1	A	1072	ARG
1	A	1076	PHE
1	A	1079	GLU
1	A	1083	LYS
1	A	1090	LYS
1	A	1093	ILE
1	A	1107	ILE
1	A	1120	ARG
1	A	1159	THR
1	A	1171	VAL
1	A	1181	LYS
1	A	1182	ARG
1	A	1183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	28	ASN
1	A	150	ASN
1	A	197	ASN
1	A	211	GLN
1	A	217	ASN
1	A	237	HIS
1	A	434	GLN
1	A	444	GLN
1	A	450	ASN
1	A	535	HIS
1	A	631	ASN
1	A	698	ASN
1	A	915	HIS
1	A	1088	GLN
1	A	1155	GLN

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	0.39	0	20,26,29	0.29	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	11	DOC	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
6	ACT	A	1304	5	3,3,3	0.98	0	3,3,3	0.67	0
4	DTP	A	1301	5	31,32,32	0.54	0	46,50,50	0.59	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	-	4/22/34/34	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

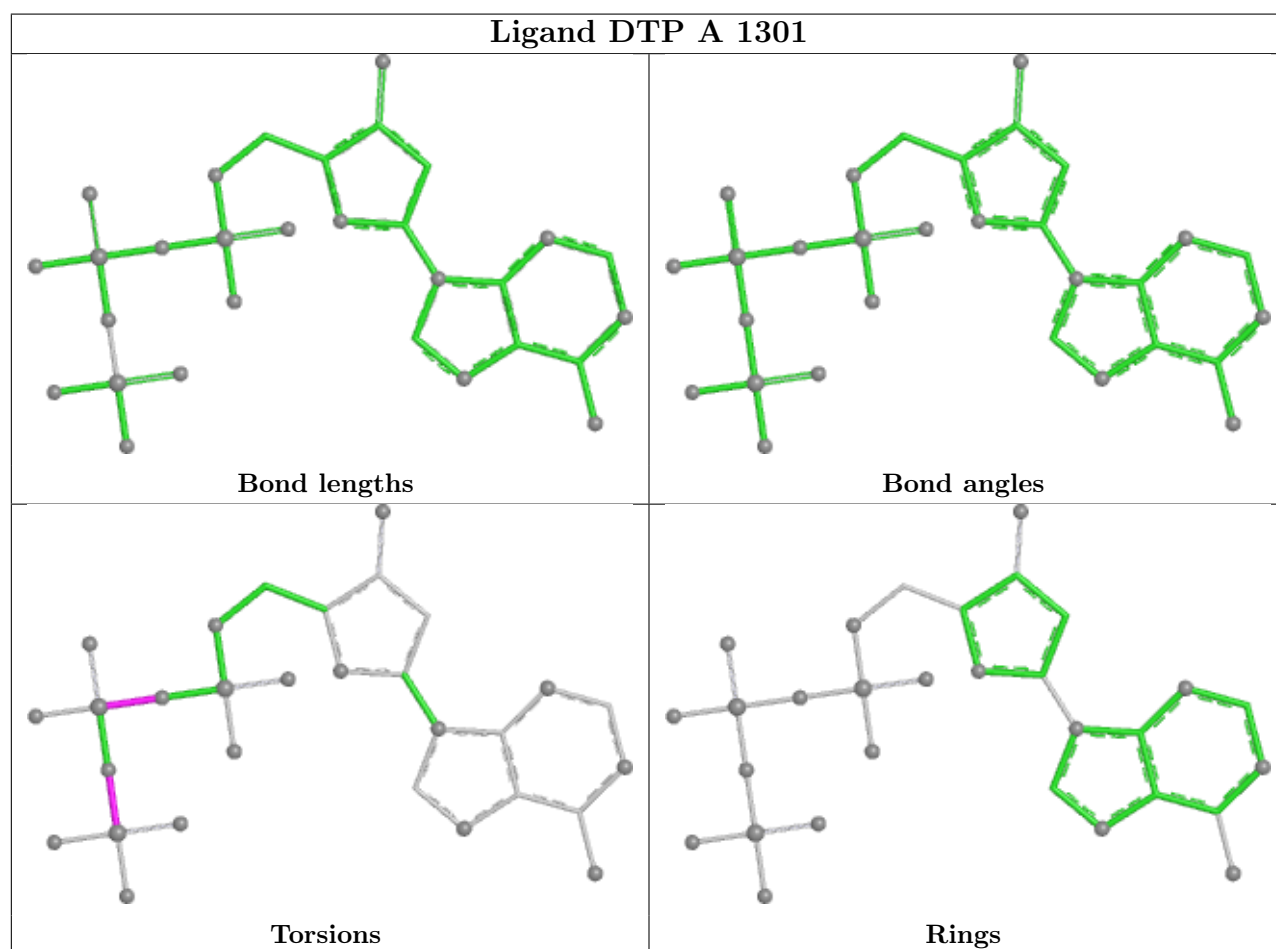
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3B-PG-O2G
4	A	1301	DTP	PB-O3B-PG-O3G
4	A	1301	DTP	PB-O3B-PG-O1G
4	A	1301	DTP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1304	ACT	3	0
4	A	1301	DTP	2	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	1122/1185 (94%)	0.27	62 (5%) 30 28	39, 76, 127, 157	0
2	P	10/11 (90%)	-0.01	1 (10%) 12 10	58, 71, 109, 125	0
3	T	15/16 (93%)	-0.21	0 100 100	43, 67, 117, 125	0
All	All	1147/1212 (94%)	0.26	63 (5%) 30 28	39, 76, 127, 157	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	4.3
1	A	218	VAL	4.2
1	A	1030	LEU	4.1
1	A	221	ASN	3.9
1	A	1184	ILE	3.9
1	A	1019	VAL	3.9
1	A	1028	ASP	3.7
1	A	1098	PHE	3.5
1	A	345	GLY	3.5
1	A	111	ASN	3.4
1	A	1035	LEU	3.4
1	A	346	PHE	3.4
1	A	215	ASN	3.3
1	A	233	VAL	3.3
1	A	677	CYS	3.2
1	A	1029	VAL	3.2
1	A	1027	LEU	3.1
1	A	1003	PHE	3.1
1	A	26	LEU	3.1
1	A	1037	LEU	3.0
1	A	1036	MET	2.9
1	A	381	PHE	2.9
1	A	1034	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	746	VAL	2.8
1	A	63	ARG	2.8
1	A	695	ASP	2.8
1	A	1140	ILE	2.7
1	A	1005	VAL	2.7
1	A	1032	SER	2.7
1	A	1016	TYR	2.7
1	A	66	ALA	2.7
1	A	984	PHE	2.6
1	A	633	LEU	2.6
1	A	1173	ARG	2.6
1	A	1012	LEU	2.6
1	A	676	THR	2.6
1	A	1145	TYR	2.6
1	A	1110	ALA	2.5
1	A	68	ASP	2.5
1	A	112	GLN	2.5
1	A	220	ARG	2.5
1	A	1015	CYS	2.5
1	A	1103	THR	2.5
1	A	749	ARG	2.4
1	A	1033	HIS	2.4
2	P	1	DT	2.3
1	A	801	SER	2.3
1	A	800	PRO	2.3
1	A	1038	GLU	2.2
1	A	1146	TYR	2.2
1	A	1150	LEU	2.2
1	A	629	ILE	2.2
1	A	1179	TRP	2.2
1	A	1102	VAL	2.2
1	A	563	ALA	2.2
1	A	1026	TRP	2.2
1	A	214	ALA	2.2
1	A	798	ILE	2.2
1	A	1137	ILE	2.2
1	A	1164	LEU	2.1
1	A	232	LYS	2.1
1	A	896	GLU	2.1
1	A	1007	LEU	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	0.96	0.10	57,68,72,73	0

6.3 Carbohydrates [i](#)

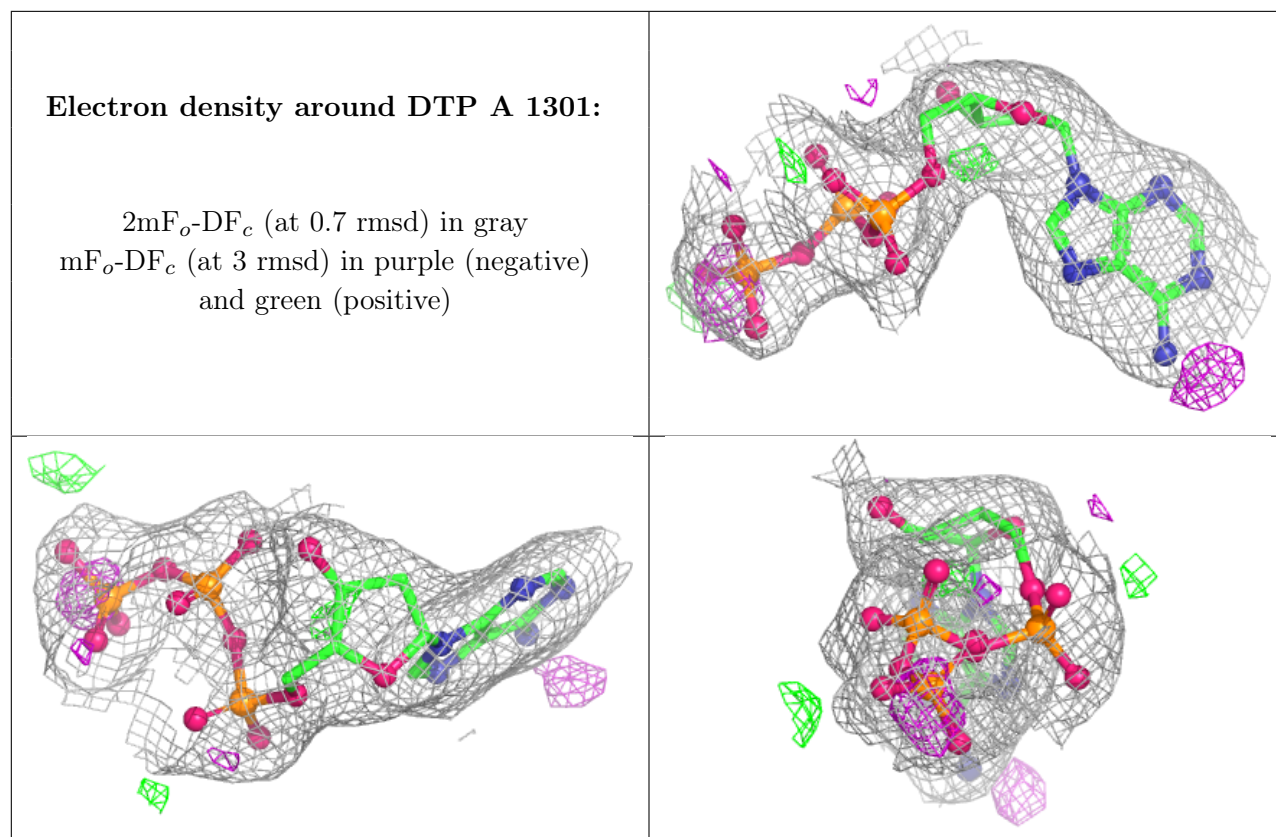
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
6	ACT	A	1304	4/4	0.94	0.10	66,67,67,70	0
4	DTP	A	1301	30/30	0.96	0.08	41,46,75,82	0
5	CA	A	1303	1/1	0.98	0.04	65,65,65,65	0
5	CA	A	1302	1/1	0.98	0.04	61,61,61,61	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.