Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID	:	8B67 / pdb_00008b67
Title	:	The crystal structure of M644G variant of DNA Pol Epsilon containing CTP in the polymerase active site
Authors	:	Parkash, V.; Johansson, E.
Deposited on	:	2022-09-26
Resolution	:	2.60 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:

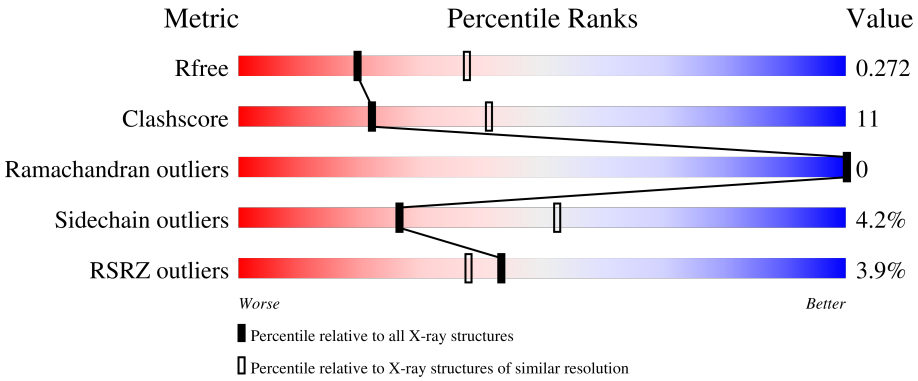
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 <=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	4% 67% 23% · 9%
2	P	11	55% 45%
3	T	16	56% 38% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9148 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	1085	Total	C	N	O	S	0	0	0
			8570	5503	1411	1613	43			

There are 6 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	644	GLY	MET	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
			217	106	38	63	10			

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

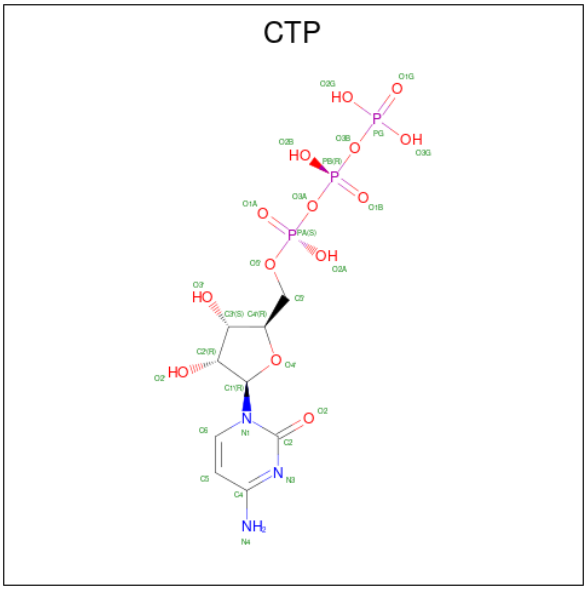
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			310	147	57	91	15			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

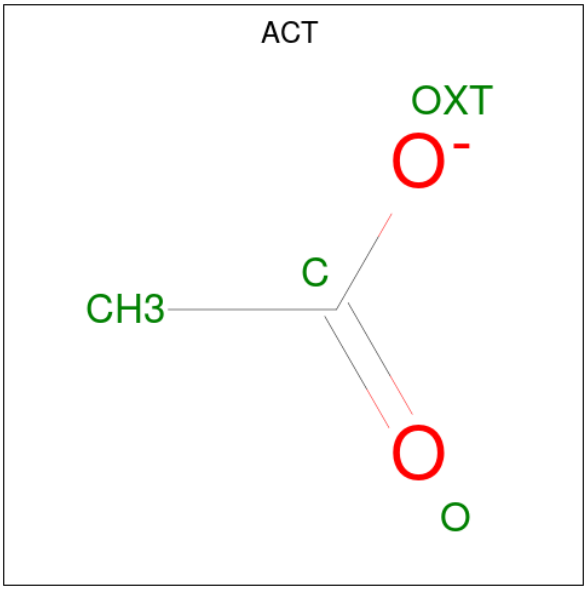
- Molecule 5 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$)

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

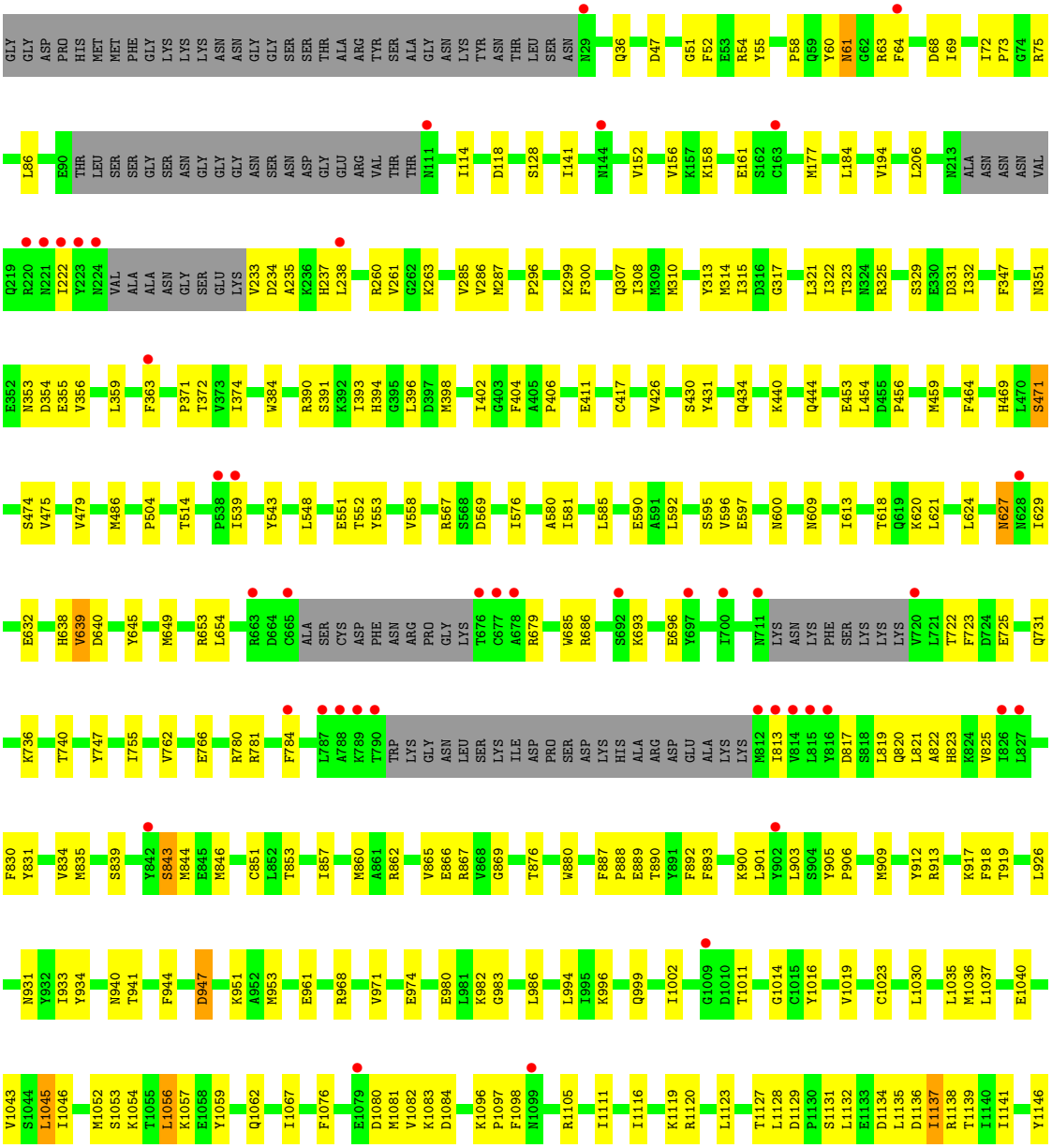
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0
7	P	1	Total O 1 1	0	0
7	T	5	Total O 5 5	0	0

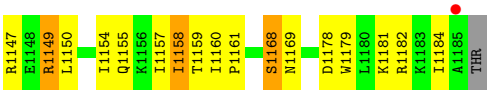
3 Residue-property plots (i)

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: DNA polymerase epsilon catalytic subunit A

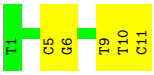
Chain A:





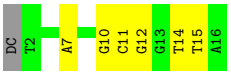
• Molecule 2: Primer DNA sequence

Chain P:



• Molecule 3: Template DNA sequence

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.06Å 67.36Å 152.13Å 90.00° 111.48° 90.00°	Depositor
Resolution (Å)	75.40 – 2.60 75.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (75.40-2.60) 98.6 (75.40-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.239 , 0.276 0.240 , 0.272	Depositor DCC
R_{free} test set	2335 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9148	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CTP, DOC, ACT, 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	0.37	0/8768	0.60	4/11898 (0.0%)
2	P	0.21	0/222	0.43	0/341
3	T	0.19	0/347	0.39	0/534
All	All	0.36	0/9337	0.59	4/12773 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	TYR	CB-CA-C	5.85	118.53	110.34
1	A	61	ASN	N-CA-C	-5.44	106.52	112.72
1	A	60	TYR	N-CA-C	-5.42	98.99	107.93
1	A	1168	SER	CB-CA-C	5.19	118.92	109.83

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	8570	0	8173	183	0
2	P	217	0	123	6	0
3	T	310	0	170	5	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	29	0	12	1	0
6	A	4	0	3	0	0
7	A	9	0	0	0	0
7	P	1	0	0	0	0
7	T	5	0	0	0	0
All	All	9148	0	8481	189	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 (189) 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:393:ILE:HG22	1:A:394:HIS:HD2	1.40	0.85
1:A:1011:THR:HG23	1:A:1014:GLY:H	1.42	0.84
1:A:296:PRO:HB2	1:A:299:LYS:HB3	1.59	0.83
1:A:1056:LEU:HD21	1:A:1067:ILE:HG23	1.58	0.83
1:A:1096:LYS:HD3	1:A:1097:PRO:HA	1.61	0.82
1:A:325:ARG:HB2	1:A:353:ASN:HA	1.62	0.82
1:A:456:PRO:HA	1:A:459:MET:HE2	1.64	0.80
1:A:551:GLU:HG2	1:A:685:TRP:HE1	1.45	0.80
2:P:10:DT:H2"	2:P:11:DOC:H5'	1.64	0.79
1:A:299:LYS:HD2	1:A:1081:MET:SD	2.21	0.79
1:A:649:MET:HE1	1:A:831:TYR:HA	1.64	0.79
1:A:354:ASP:OD1	1:A:355:GLU:N	2.17	0.76
1:A:552:THR:HG22	1:A:553:TYR:H	1.50	0.75
1:A:905:TYR:O	1:A:909:MET:HG2	1.86	0.75
1:A:1120:ARG:HG3	1:A:1135:LEU:HD11	1.68	0.74
1:A:834:VAL:HG12	1:A:843:SER:H	1.56	0.70
1:A:953:MET:HG3	1:A:971:VAL:HG22	1.72	0.70
1:A:649:MET:HE2	1:A:846:MET:HE2	1.72	0.70
1:A:1052:MET:HE1	1:A:1056:LEU:HG	1.75	0.69
1:A:1127:THR:HG21	1:A:1132:LEU:HD22	1.76	0.68
1:A:323:THR:HG21	1:A:332:ILE:HD12	1.77	0.67
1:A:1127:THR:HG23	1:A:1129:ASP:H	1.58	0.67
1:A:543:TYR:HB2	1:A:548:LEU:HD11	1.78	0.66
1:A:876:THR:HB	2:P:11:DOC:H3'2	1.78	0.65
1:A:784:PHE:HB3	1:A:820:GLN:HB3	1.78	0.64
1:A:860:MET:HE2	1:A:918:PHE:HE2	1.60	0.64
1:A:968:ARG:HG2	1:A:983:GLY:HA3	1.80	0.64
1:A:1123:LEU:O	1:A:1127:THR:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:THR:HG22	1:A:553:TYR:N	2.13	0.63
1:A:551:GLU:HG2	1:A:685:TRP:NE1	2.11	0.63
1:A:310:MET:SD	1:A:474:SER:OG	2.55	0.63
1:A:1097:PRO:HD2	1:A:1105:ARG:HG2	1.80	0.62
1:A:299:LYS:NZ	1:A:1080:ASP:HB2	2.15	0.62
1:A:780:ARG:HB3	1:A:823:HIS:CD2	2.35	0.61
1:A:1149:ARG:HE	3:T:12:DG:H5"	1.65	0.61
1:A:580:ALA:HA	1:A:867:ARG:HH21	1.65	0.61
1:A:693:LYS:N	1:A:696:GLU:OE1	2.33	0.61
1:A:475:VAL:O	1:A:479:VAL:HG23	2.01	0.60
1:A:371:PRO:HG2	1:A:374:ILE:HD11	1.82	0.60
1:A:892:PHE:HD1	1:A:900:LYS:HB3	1.66	0.60
1:A:152:VAL:O	1:A:156:VAL:HG23	2.01	0.60
1:A:1178:ASP:O	1:A:1182:ARG:HG3	2.02	0.59
1:A:819:LEU:O	1:A:822:ALA:HB3	2.02	0.59
1:A:1096:LYS:HD3	1:A:1098:PHE:H	1.66	0.59
1:A:817:ASP:O	1:A:820:GLN:HG3	2.04	0.57
1:A:585:LEU:HD22	1:A:618:THR:HG23	1.86	0.57
1:A:679:ARG:HB3	1:A:762:VAL:HB	1.86	0.57
1:A:1040:GLU:O	1:A:1043:VAL:HG12	2.04	0.57
1:A:951:LYS:HB2	1:A:974:GLU:HA	1.86	0.57
1:A:653:ARG:NH2	1:A:766:GLU:O	2.37	0.56
1:A:1046:ILE:HD11	1:A:1146:TYR:CG	2.41	0.56
1:A:1155:GLN:HA	1:A:1159:THR:OG1	2.05	0.55
1:A:285:VAL:HB	1:A:371:PRO:HA	1.88	0.55
1:A:1080:ASP:O	1:A:1083:LYS:HG2	2.06	0.55
1:A:1134:ASP:OD2	1:A:1139:THR:HG21	2.06	0.55
1:A:1137:ILE:HG22	1:A:1141:ILE:HG13	1.88	0.55
1:A:440:LYS:O	1:A:444:GLN:HG3	2.07	0.54
1:A:1082:VAL:HG12	1:A:1082:VAL:O	2.07	0.54
1:A:926:LEU:HG	1:A:934:TYR:CE1	2.43	0.54
1:A:931:ASN:HB2	1:A:933:ILE:HD13	1.90	0.54
1:A:299:LYS:HG3	1:A:300:PHE:N	2.22	0.54
1:A:567:ARG:NH2	1:A:569:ASP:OD2	2.41	0.54
1:A:834:VAL:HG12	1:A:843:SER:N	2.23	0.53
1:A:51:GLY:O	1:A:128:SER:OG	2.26	0.53
1:A:393:ILE:HG22	1:A:394:HIS:CD2	2.31	0.53
1:A:58:PRO:HG2	1:A:73:PRO:HB2	1.91	0.53
1:A:329:SER:HB3	1:A:464:PHE:HA	1.91	0.53
1:A:1096:LYS:HG2	1:A:1098:PHE:CD1	2.43	0.53
1:A:36:GLN:HB3	1:A:86:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:NH1	1:A:331:ASP:OD1	2.42	0.53
1:A:893:PHE:CZ	1:A:903:LEU:HD22	2.44	0.53
1:A:620:LYS:HB2	1:A:888:PRO:HG3	1.90	0.52
1:A:649:MET:HA	1:A:654:LEU:HD12	1.92	0.52
1:A:356:VAL:HG22	1:A:394:HIS:ND1	2.24	0.52
1:A:596:VAL:HG23	1:A:597:GLU:HG3	1.92	0.52
1:A:999:GLN:HA	1:A:1002:ILE:HG22	1.92	0.52
1:A:817:ASP:HA	1:A:820:GLN:HG2	1.91	0.52
1:A:308:ILE:HD12	1:A:359:LEU:HD21	1.92	0.51
1:A:299:LYS:HA	1:A:1081:MET:SD	2.51	0.51
1:A:374:ILE:HD13	1:A:417:CYS:SG	2.50	0.51
1:A:1059:TYR:O	1:A:1062:GLN:HB2	2.11	0.51
1:A:609:ASN:ND2	1:A:613:ILE:HD11	2.26	0.51
1:A:645:TYR:HB2	5:A:1304:CTP:O3'	2.11	0.51
1:A:1127:THR:HG23	1:A:1129:ASP:N	2.26	0.50
1:A:576:ILE:HG21	1:A:581:ILE:HD11	1.93	0.50
1:A:986:LEU:HA	1:A:996:LYS:HG2	1.94	0.49
1:A:234:ASP:HB3	1:A:237:HIS:ND1	2.27	0.49
1:A:552:THR:HG23	3:T:7:DA:OP1	2.12	0.49
1:A:286:VAL:HG11	1:A:486:MET:SD	2.53	0.49
1:A:434:GLN:HB2	2:P:9:DT:OP2	2.11	0.49
1:A:906:PRO:HA	1:A:909:MET:SD	2.53	0.49
1:A:552:THR:CG2	1:A:553:TYR:H	2.21	0.49
1:A:363:PHE:CZ	1:A:398:MET:HG3	2.47	0.49
1:A:722:THR:HG22	1:A:725:GLU:OE1	2.13	0.49
1:A:982:LYS:HB3	2:P:10:DT:H5"	1.95	0.49
1:A:581:ILE:HG21	1:A:621:LEU:O	2.12	0.49
1:A:638:HIS:HB3	1:A:947:ASP:HB2	1.95	0.48
1:A:1127:THR:O	1:A:1128:LEU:HB2	2.14	0.48
1:A:1181:LYS:O	1:A:1184:ILE:HG13	2.13	0.48
1:A:323:THR:OG1	1:A:351:ASN:HA	2.14	0.48
1:A:158:LYS:O	1:A:161:GLU:HG3	2.14	0.47
1:A:679:ARG:HA	1:A:679:ARG:HD2	1.74	0.47
1:A:580:ALA:CA	1:A:867:ARG:HH21	2.27	0.47
1:A:865:VAL:O	1:A:869:GLY:N	2.48	0.47
1:A:1147:ARG:HH11	1:A:1147:ARG:HG3	1.80	0.47
1:A:54:ARG:NH2	1:A:118:ASP:OD1	2.48	0.47
1:A:141:ILE:HD11	1:A:206:LEU:HD21	1.97	0.47
1:A:980:GLU:HB3	1:A:982:LYS:HE2	1.97	0.47
1:A:1149:ARG:HG2	1:A:1149:ARG:NH1	2.30	0.47
1:A:913:ARG:O	1:A:917:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:CB	1:A:86:LEU:HD12	2.45	0.46
1:A:1097:PRO:O	1:A:1105:ARG:HD3	2.15	0.46
1:A:299:LYS:HG3	1:A:300:PHE:H	1.80	0.46
1:A:600:ASN:HB3	1:A:901:LEU:HD13	1.96	0.46
3:T:10:DG:C8	3:T:10:DG:H5'	2.50	0.46
3:T:14:DT:H2'	3:T:15:DT:C6	2.50	0.46
1:A:260:ARG:HB2	1:A:263:LYS:HD2	1.98	0.46
1:A:55:TYR:CZ	1:A:75:ARG:HB2	2.51	0.46
1:A:1096:LYS:HB3	1:A:1127:THR:OG1	2.16	0.45
1:A:177:MET:HE2	1:A:184:LEU:HB3	1.97	0.45
1:A:620:LYS:O	1:A:624:LEU:HD13	2.16	0.45
1:A:590:GLU:HB3	1:A:912:TYR:CE2	2.52	0.45
1:A:887:PHE:CE2	1:A:906:PRO:HG3	2.52	0.45
1:A:1083:LYS:HG3	1:A:1084:ASP:N	2.32	0.45
1:A:314:MET:HE2	1:A:317:GLY:HA2	1.97	0.45
1:A:1160:ILE:N	1:A:1161:PRO:CD	2.80	0.45
1:A:69:ILE:HA	1:A:72:ILE:HD12	1.98	0.45
1:A:821:LEU:O	1:A:825:VAL:HG23	2.17	0.45
1:A:880:TRP:HB3	1:A:953:MET:HE1	1.98	0.45
1:A:1096:LYS:HG2	1:A:1098:PHE:HD1	1.82	0.45
1:A:310:MET:HE2	1:A:321:LEU:HD11	1.98	0.44
1:A:835:MET:SD	1:A:844:MET:HA	2.57	0.44
1:A:1111:ILE:O	1:A:1119:LYS:HG3	2.16	0.44
1:A:1037:LEU:O	1:A:1138:ARG:NH2	2.50	0.44
1:A:1149:ARG:HG2	1:A:1149:ARG:HH11	1.82	0.44
1:A:287:MET:HG3	1:A:315:ILE:HG13	1.99	0.44
1:A:347:PHE:CE2	1:A:475:VAL:HG12	2.52	0.44
1:A:64:PHE:CD1	1:A:64:PHE:N	2.86	0.44
1:A:1134:ASP:O	1:A:1135:LEU:HD23	2.17	0.44
3:T:11:DC:H2"	3:T:12:DG:C8	2.52	0.44
1:A:569:ASP:OD1	1:A:569:ASP:N	2.49	0.44
1:A:1157:ILE:C	1:A:1158:ILE:HG12	2.43	0.44
1:A:1136:ASP:HB3	1:A:1139:THR:HG23	1.99	0.44
1:A:781:ARG:HB2	1:A:823:HIS:HB3	2.00	0.43
1:A:313:TYR:HE1	1:A:322:ILE:HG13	1.83	0.43
1:A:426:VAL:HA	1:A:430:SER:HB3	1.98	0.43
1:A:736:LYS:O	1:A:740:THR:OG1	2.33	0.43
1:A:994:LEU:HA	1:A:1045:LEU:CD2	2.48	0.43
1:A:592:LEU:HD12	1:A:592:LEU:HA	1.79	0.43
1:A:471:SER:O	1:A:475:VAL:HG22	2.19	0.43
1:A:390:ARG:HD2	1:A:390:ARG:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ARG:O	1:A:866:GLU:HG2	2.19	0.43
1:A:627:ASN:H	1:A:627:ASN:ND2	2.17	0.43
1:A:627:ASN:H	1:A:627:ASN:HD22	1.66	0.43
1:A:1158:ILE:C	1:A:1161:PRO:HD2	2.43	0.43
1:A:1123:LEU:HD13	1:A:1135:LEU:HD22	2.00	0.43
1:A:307:GLN:HG2	1:A:390:ARG:HH21	1.83	0.42
1:A:391:SER:HB2	1:A:396:LEU:HB2	2.01	0.42
1:A:553:TYR:HE2	1:A:835:MET:HG3	1.84	0.42
1:A:1168:SER:O	1:A:1169:ASN:C	2.62	0.42
1:A:454:LEU:HD11	1:A:469:HIS:HD2	1.85	0.42
1:A:1016:TYR:HA	1:A:1019:VAL:HG12	2.01	0.42
2:P:5:DC:H2"	2:P:6:DG:C8	2.55	0.42
1:A:299:LYS:HZ2	1:A:1080:ASP:HB2	1.83	0.42
1:A:406:PRO:HA	1:A:411:GLU:O	2.20	0.42
1:A:696:GLU:OE2	1:A:747:TYR:OH	2.26	0.42
1:A:994:LEU:HA	1:A:1045:LEU:HD23	2.01	0.42
1:A:552:THR:CG2	1:A:553:TYR:N	2.80	0.42
1:A:931:ASN:HB2	1:A:933:ILE:CD1	2.50	0.42
1:A:47:ASP:HB3	1:A:52:PHE:HB2	2.01	0.41
1:A:299:LYS:HZ1	1:A:1080:ASP:HB2	1.83	0.41
1:A:1052:MET:HE2	1:A:1059:TYR:CD2	2.55	0.41
1:A:1150:LEU:O	1:A:1154:ILE:HG13	2.21	0.41
1:A:261:VAL:HG11	1:A:504:PRO:HD3	2.03	0.41
1:A:645:TYR:HE2	1:A:851:CYS:SG	2.43	0.41
2:P:5:DC:H2"	2:P:6:DG:H5'	2.03	0.41
1:A:68:ASP:O	1:A:72:ILE:HD12	2.21	0.41
1:A:961:GLU:HB2	1:A:1179:TRP:CD2	2.56	0.41
1:A:1116:ILE:H	1:A:1116:ILE:HG12	1.74	0.41
1:A:235:ALA:HA	1:A:238:LEU:CD1	2.51	0.41
1:A:639:VAL:HG13	1:A:944:PHE:CD1	2.56	0.41
1:A:723:PHE:CZ	1:A:731:GLN:HB3	2.56	0.40
1:A:1023:CYS:HB3	1:A:1154:ILE:HD13	2.03	0.40
1:A:686:ARG:HG3	1:A:755:ILE:HG12	2.03	0.40
1:A:889:GLU:HB3	1:A:890:THR:H	1.78	0.40
1:A:919:THR:HA	1:A:940:ASN:HD22	1.86	0.40
1:A:402:ILE:HD12	1:A:404:PHE:CD2	2.56	0.40
1:A:853:THR:O	1:A:857:ILE:HG13	2.22	0.40
1:A:374:ILE:HG21	1:A:384:TRP:HZ2	1.87	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	1071/1191 (90%)	1036 (97%)	35 (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
1	A	904/1066 (85%)	866 (96%)	38 (4%)	26 52

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	63	ARG
1	A	114	ILE
1	A	194	VAL
1	A	222	ILE
1	A	233	VAL
1	A	372	THR
1	A	431	TYR
1	A	453	GLU
1	A	471	SER
1	A	514	THR
1	A	539	ILE
1	A	558	VAL

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Mol	Chain	Res	Type
1	A	595	SER
1	A	627	ASN
1	A	629	ILE
1	A	632	GLU
1	A	639	VAL
1	A	640	ASP
1	A	813	ILE
1	A	830	PHE
1	A	839	SER
1	A	843	SER
1	A	941	THR
1	A	947	ASP
1	A	1030	LEU
1	A	1035	LEU
1	A	1036	MET
1	A	1045	LEU
1	A	1053	SER
1	A	1054	LYS
1	A	1056	LEU
1	A	1057	LYS
1	A	1076	PHE
1	A	1131	SER
1	A	1137	ILE
1	A	1149	ARG
1	A	1158	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	168	GLN
1	A	197	ASN
1	A	365	HIS
1	A	469	HIS
1	A	627	ASN
1	A	915	HIS
1	A	940	ASN
1	A	993	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)

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	0.43	0	20,26,29	0.37	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 2 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	1305	4	3,3,3	1.40	1 (33%)	3,3,3	1.30	0
5	CTP	A	1304	4	29,30,30	0.59	0	43,47,47	0.61	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
5	CTP	A	1304	4	-	4/22/38/38	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1305	ACT	CH3-C	2.02	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

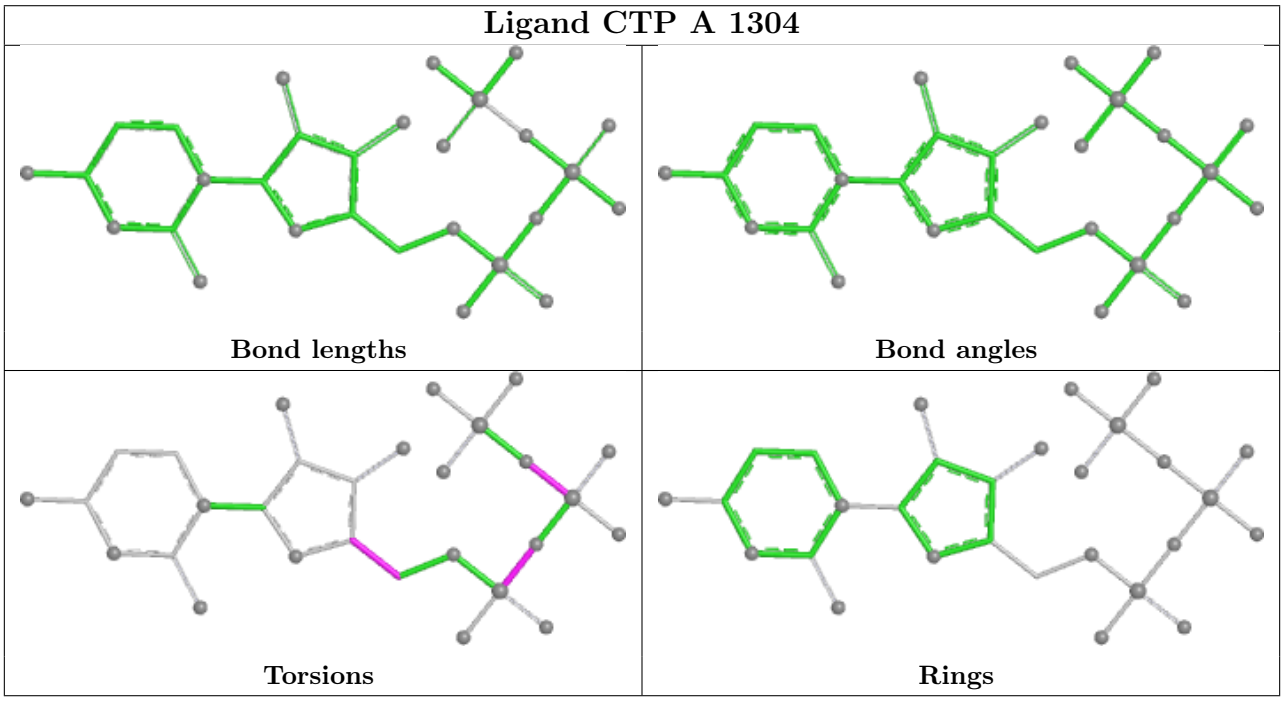
Mol	Chain	Res	Type	Atoms
5	A	1304	CTP	O4'-C4'-C5'-O5'
5	A	1304	CTP	PG-O3B-PB-O2B
5	A	1304	CTP	PB-O3A-PA-O2A
5	A	1304	CTP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1304	CTP	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 then 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	1085/1191 (91%)	0.46	43 (3%) 42 37	21, 55, 86, 110	0
2	P	10/11 (90%)	-0.26	0 100 100	33, 43, 55, 58	0
3	T	15/16 (93%)	-0.08	0 100 100	30, 38, 90, 112	0
All	All	1110/1218 (91%)	0.44	43 (3%) 43 38	21, 54, 86, 112	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	CYS	5.5
1	A	720	VAL	5.3
1	A	64	PHE	4.4
1	A	539	ILE	4.3
1	A	678	ALA	4.1
1	A	700	ILE	4.0
1	A	222	ILE	3.7
1	A	29	ASN	3.6
1	A	223	TYR	3.3
1	A	711	ASN	3.1
1	A	111	ASN	3.0
1	A	788	ALA	3.0
1	A	677	CYS	3.0
1	A	815	LEU	3.0
1	A	816	TYR	2.9
1	A	224	ASN	2.9
1	A	1099	ASN	2.8
1	A	787	LEU	2.8
1	A	538	PRO	2.8
1	A	628	ASN	2.7
1	A	812	MET	2.7
1	A	790	THR	2.5
1	A	813	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	2.4
1	A	842	TYR	2.4
1	A	1185	ALA	2.4
1	A	1079	GLU	2.3
1	A	902	TYR	2.3
1	A	784	PHE	2.3
1	A	163	CYS	2.2
1	A	676	THR	2.2
1	A	1009	GLY	2.2
1	A	697	TYR	2.2
1	A	363	PHE	2.2
1	A	221	ASN	2.2
1	A	238	LEU	2.2
1	A	827	LEU	2.1
1	A	692	SER	2.1
1	A	814	VAL	2.1
1	A	789	LYS	2.1
1	A	220	ARG	2.1
1	A	826	ILE	2.1
1	A	663	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, 95^{th} 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	0.95	0.10	18,23,36,43	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

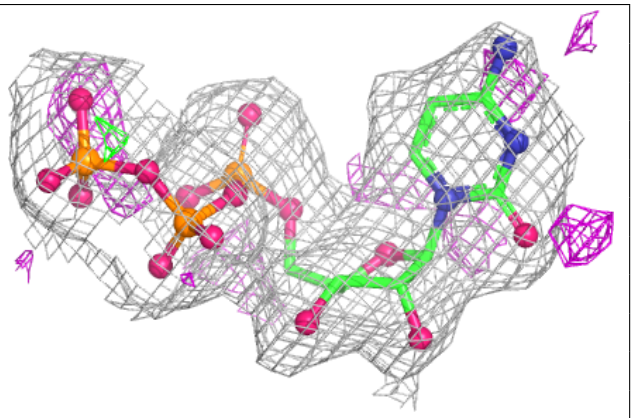
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

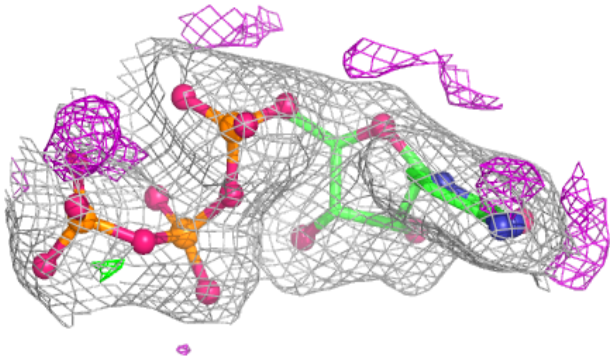
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	1302	1/1	0.65	0.16	88,88,88,88	0
6	ACT	A	1305	4/4	0.77	0.16	47,66,68,76	0
4	CA	A	1303	1/1	0.94	0.06	65,65,65,65	0
5	CTP	A	1304	29/29	0.95	0.08	18,30,40,52	0
4	CA	A	1301	1/1	0.99	0.06	33,33,33,33	0

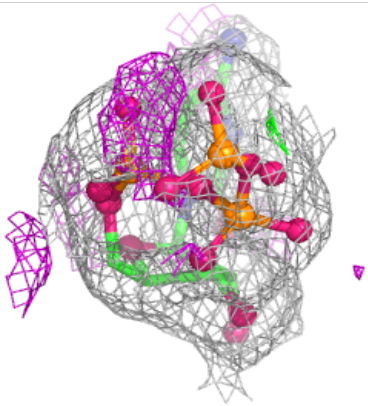
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CTP A 1304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.