



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 6QCV / pdb_00006qcv
Title : Crystal structure of influenza B polymerase initiation state with capped 14-mer RNA primer and CTP
Authors : Cusack, S.; Drncova, P.
Deposited on : 2018-12-31
Resolution : 3.24 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:

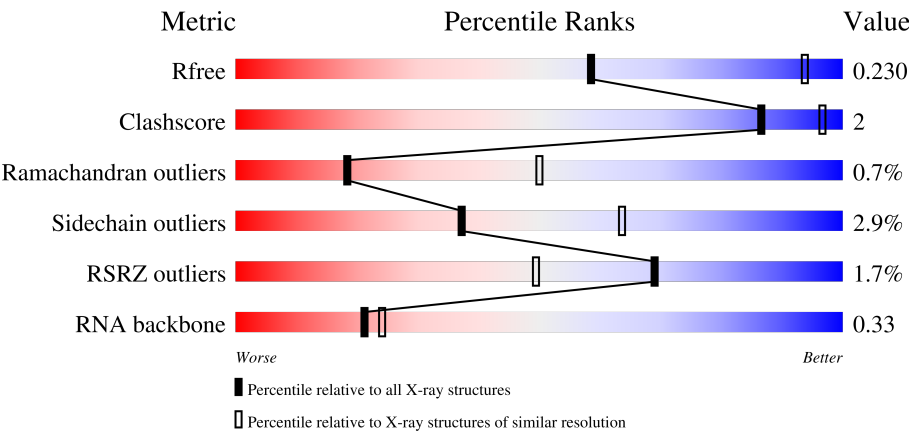
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.24 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.



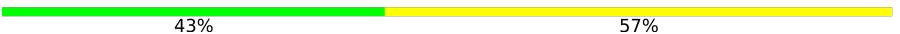
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)
RNA backbone	3983	1047 (3.52-2.96)

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	751	2% 87% 8% 5%
2	B	772	2% 89% 7% ...
3	C	798	2% 83% 8% 8%
4	M	15	13% 60% 27% 13%

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Mol	Chain	Length	Quality of chain
5	R	21	 67% 29% 5%
6	V	14	 43% 57%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18569 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5755	3657	963	1095	40			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	746	Total	C	N	O	S	0	0	0
			5852	3692	1016	1092	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	733	Total	C	N	O	S	0	0	0
			5863	3726	1026	1071	40			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	GLY	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3

- Molecule 4 is a RNA chain called RNA (5'-D(*(GDM))-R(P*GP*AP*AP*UP*GP*CP*UP*AP*UP*AP*AP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	15	Total	C	N	O	P	0	0	0
			330	146	61	107	16			

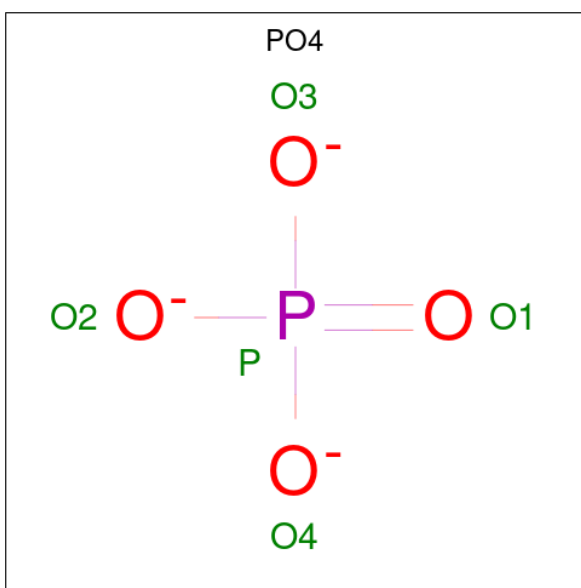
- Molecule 5 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP*CP*UP*AP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	21	Total	C	N	O	P	0	0	0
			427	193	63	151	20			

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*G)-3').

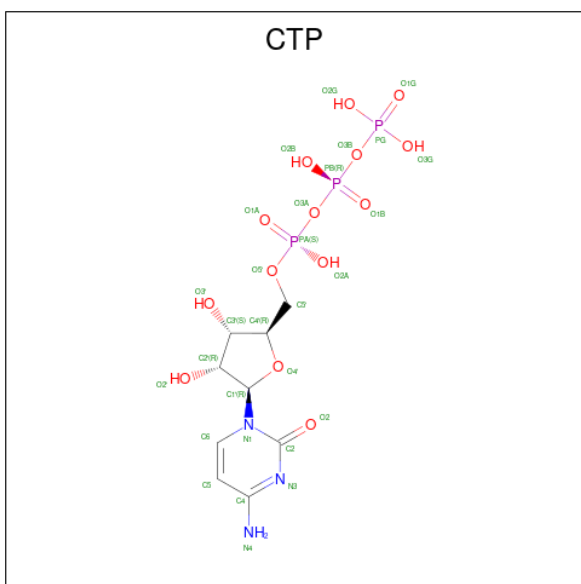
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	V	14	Total	C	N	O	P	0	0	0
			307	137	62	94	14			

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

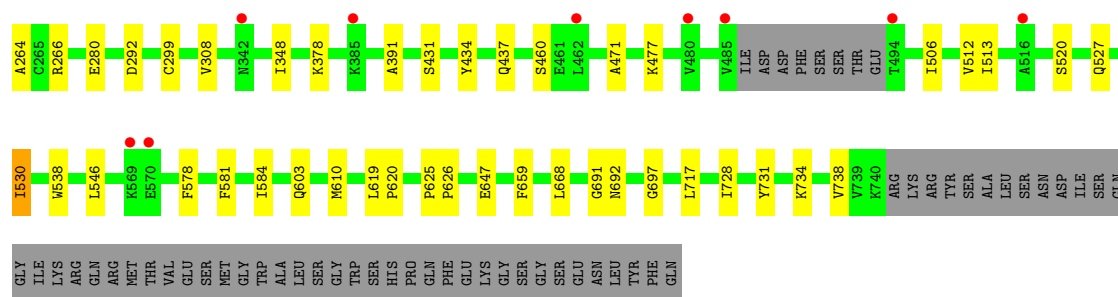
- Molecule 8 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



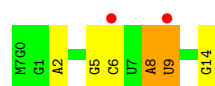
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	
			29	9	3	14	3	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

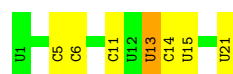
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		



- Molecule 4: RNA (5'-D(*(GDM))-R(P*GP*AP*AP*UP*GP*CP*UP*AP*UP*AP*AP*UP*A P*G)-3')



- Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP *CP*UP*AP*UP*U)-3')



- Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.19Å 200.19Å 256.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.24 50.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	67.7 (50.00-3.24) 67.6 (50.00-3.24)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.234 0.207 , 0.230	Depositor DCC
R_{free} test set	3069 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18569	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: CTP, MG, PO4, M7G

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	1.01	0/5871	1.48	2/7918 (0.0%)
2	B	1.02	0/5967	1.49	2/8043 (0.0%)
3	C	1.03	0/5963	1.44	2/8014 (0.0%)
4	M	0.35	0/337	0.66	0/523
5	R	0.34	0/473	0.69	1/732 (0.1%)
6	V	0.37	0/345	0.69	0/535
All	All	0.99	0/18956	1.43	7/25765 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	348	ILE	CA-C-N	5.65	126.36	120.03
3	C	348	ILE	C-N-CA	5.65	126.36	120.03
5	R	13	U	C2'-C3'-O3'	5.40	117.60	109.50
2	B	524	ILE	CA-C-N	5.14	125.79	120.03
2	B	524	ILE	C-N-CA	5.14	125.79	120.03
1	A	191	ILE	CA-C-N	5.10	124.81	119.92
1	A	191	ILE	C-N-CA	5.10	124.81	119.92

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	5755	0	5730	28	0
2	B	5852	0	5872	28	0
3	C	5863	0	6031	26	0
4	M	330	0	167	2	0
5	R	427	0	219	2	0
6	V	307	0	153	1	0
7	A	5	0	0	0	0
8	B	29	0	12	0	0
9	B	1	0	0	0	0
All	All	18569	0	18184	77	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 2.

All (77) 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:467:ASN:HA	3:C:54:CYS:SG	2.39	0.63
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.84	0.59
1:A:356:LEU:HD13	1:A:478:VAL:HG23	1.85	0.58
1:A:574:ARG:HB3	2:B:549:LEU:HD22	1.86	0.57
1:A:386:MET:O	2:B:380:ARG:NH1	2.40	0.54
1:A:593:SER:HB3	3:C:241:ASN:HB3	1.93	0.50
2:B:370:CYS:HA	2:B:373:LEU:HD13	1.94	0.50
2:B:170:ILE:O	2:B:173:SER:OG	2.28	0.50
1:A:546:VAL:HG12	1:A:549:ARG:HB2	1.93	0.50
3:C:80:LYS:HA	3:C:93:CYS:HA	1.94	0.49
3:C:728:ILE:HD13	3:C:738:VAL:HB	1.95	0.49
2:B:26:GLY:O	2:B:233:ARG:NH2	2.45	0.49
3:C:731:TYR:CE2	3:C:734:LYS:HG3	2.48	0.49
5:R:21:U:O2	5:R:21:U:O4'	2.30	0.49
1:A:642:MET:HG3	1:A:695:TRP:CZ3	2.48	0.48
3:C:264:ALA:HB2	3:C:530:ILE:HD11	1.96	0.48
2:B:241:ILE:HG22	2:B:410:MET:HG2	1.95	0.48
3:C:717:LEU:HD21	3:C:728:ILE:HD11	1.96	0.48
2:B:282:LEU:HD22	2:B:440:LEU:HD13	1.96	0.47
1:A:610:ASN:HD22	1:A:610:ASN:N	2.13	0.47
3:C:581:PHE:O	3:C:584:ILE:HG13	2.15	0.47
1:A:226:MET:HE1	2:B:319:LEU:HD23	1.96	0.47
3:C:659:PHE:CZ	3:C:668:LEU:HD11	2.50	0.46
3:C:603:GLN:OE1	3:C:697:GLY:N	2.47	0.46
1:A:36:PHE:CZ	1:A:181:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:603:GLN:NE2	3:C:692:ASN:O	2.49	0.46
1:A:483:ASN:HB3	1:A:497:TYR:HE2	1.80	0.45
4:M:8:A:O2'	4:M:9:U:OP1	2.27	0.45
3:C:258:SER:O	3:C:261:MET:HB3	2.17	0.45
1:A:410:LEU:HA	1:A:450:LYS:HB3	1.98	0.45
2:B:327:ARG:HA	2:B:334:ARG:NH1	2.32	0.45
3:C:578:PHE:CD1	3:C:620:PRO:HA	2.52	0.45
1:A:280:ASN:HD21	1:A:694:PRO:HD3	1.82	0.44
1:A:644:TYR:HA	2:B:26:GLY:HA2	2.00	0.44
2:B:508:LEU:HB3	2:B:509:PRO:HD3	2.00	0.44
1:A:242:ASN:ND2	2:B:87:CYS:SG	2.91	0.44
3:C:58:PRO:HD2	3:C:94:SER:HA	1.99	0.44
1:A:80:ILE:HA	1:A:83:MET:HE2	2.00	0.43
2:B:238:ARG:HA	2:B:238:ARG:NE	2.32	0.43
3:C:506:ILE:HG22	3:C:512:VAL:HG12	2.00	0.43
1:A:408:ASN:HA	2:B:3:ILE:HD12	2.00	0.43
3:C:89:LYS:HA	3:C:89:LYS:HE2	2.00	0.43
3:C:431:SER:HB3	3:C:434:TYR:HB2	2.01	0.43
1:A:501:VAL:CG2	1:A:517:VAL:HB	2.49	0.43
2:B:263:CYS:HA	2:B:266:LEU:HD12	2.01	0.42
1:A:438:ARG:HA	1:A:600:THR:HG21	2.01	0.42
3:C:538:TRP:CZ3	3:C:546:LEU:HD23	2.54	0.42
3:C:53:MET:SD	3:C:95:ILE:HG21	2.60	0.42
3:C:266:ARG:CZ	3:C:520:SER:HB3	2.49	0.42
1:A:533:TRP:N	1:A:534:PRO:CD	2.82	0.42
1:A:83:MET:HE1	1:A:91:VAL:HG21	2.02	0.41
2:B:628:ASN:HD22	2:B:662:THR:HG22	1.85	0.41
1:A:343:CYS:SG	1:A:501:VAL:HG13	2.60	0.41
1:A:672:LYS:O	1:A:673:GLY:C	2.62	0.41
6:V:8:A:H2'	6:V:9:C:C6	2.55	0.41
3:C:163:ASN:HD22	3:C:178:ARG:HG3	1.85	0.41
1:A:446:ILE:O	1:A:449:CYS:SG	2.78	0.41
2:B:303:THR:HG23	2:B:490:GLU:O	2.21	0.41
1:A:343:CYS:HA	1:A:478:VAL:HG21	2.03	0.41
2:B:164:ILE:N	2:B:165:PRO:HD2	2.36	0.41
5:R:5:C:H4'	5:R:6:C:OP2	2.21	0.41
2:B:266:LEU:HD13	2:B:422:VAL:HG11	2.03	0.41
2:B:444:ASP:OD1	4:M:14:G:O3'	2.37	0.41
1:A:272:HIS:HA	1:A:398:ARG:HD3	2.03	0.41
3:C:619:LEU:HB3	3:C:620:PRO:HD3	2.02	0.41
1:A:279:TYR:CE1	1:A:281:ALA:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:SER:O	1:A:505:SER:OG	2.35	0.41
2:B:40:ILE:HG21	2:B:388:LYS:HB3	2.03	0.41
2:B:370:CYS:N	2:B:371:PRO:CD	2.84	0.41
2:B:437:TRP:CD1	2:B:437:TRP:C	2.98	0.41
2:B:508:LEU:N	2:B:509:PRO:CD	2.84	0.41
3:C:625:PRO:HA	3:C:626:PRO:HD3	1.98	0.41
2:B:393:LYS:HB3	2:B:394:PRO:HD3	2.02	0.40
2:B:671:ARG:HB3	3:C:86:ILE:HD11	2.04	0.40
3:C:61:LEU:HD21	3:C:93:CYS:HB3	2.02	0.40
2:B:488:MET:HE3	2:B:497:ARG:HG3	2.04	0.40
3:C:120:PHE:O	3:C:123:ARG:HB3	2.22	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	713/751 (95%)	653 (92%)	57 (8%)	3 (0%)	30 60
2	B	742/772 (96%)	690 (93%)	47 (6%)	5 (1%)	18 50
3	C	729/798 (91%)	671 (92%)	51 (7%)	7 (1%)	12 42
All	All	2184/2321 (94%)	2014 (92%)	155 (7%)	15 (1%)	18 50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	SER
1	A	673	GLY
2	B	194	LYS
3	C	471	ALA
2	B	643	ASP
2	B	679	ARG

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Mol	Chain	Res	Type
3	C	391	ALA
3	C	477	LYS
3	C	691	GLY
3	C	292	ASP
1	A	528	VAL
2	B	410	MET
3	C	460	SER
2	B	534	ILE
3	C	308	VAL

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	638/664 (96%)	619 (97%)	19 (3%)	36	63
2	B	640/657 (97%)	623 (97%)	17 (3%)	39	65
3	C	640/694 (92%)	620 (97%)	20 (3%)	35	62
All	All	1918/2015 (95%)	1862 (97%)	56 (3%)	37	63

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	208	ILE
1	A	243	LEU
1	A	257	LEU
1	A	305	LEU
1	A	326	MET
1	A	339	LEU
1	A	356	LEU
1	A	370	LEU
1	A	382	ASP
1	A	384	GLU
1	A	405	THR
1	A	412	THR

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Mol	Chain	Res	Type
1	A	485	VAL
1	A	514	VAL
1	A	590	GLN
1	A	608	ARG
1	A	610	ASN
1	A	721	ASP
2	B	94	ARG
2	B	164	ILE
2	B	187	ILE
2	B	239	ARG
2	B	248	ILE
2	B	268	GLN
2	B	373	LEU
2	B	444	ASP
2	B	459	MET
2	B	488	MET
2	B	493	SER
2	B	533	MET
2	B	614	LEU
2	B	645	THR
2	B	666	ARG
2	B	668	LYS
2	B	671	ARG
3	C	34	ARG
3	C	50	LYS
3	C	61	LEU
3	C	62	THR
3	C	89	LYS
3	C	136	THR
3	C	173	GLU
3	C	178	ARG
3	C	229	GLU
3	C	238	GLN
3	C	259	GLN
3	C	280	GLU
3	C	299	CYS
3	C	378	LYS
3	C	437	GLN
3	C	513	ILE
3	C	527	GLN
3	C	530	ILE
3	C	610	MET

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Mol	Chain	Res	Type
3	C	647	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	268	GLN
2	B	292	ASN
2	B	628	ASN
2	B	745	HIS
3	C	11	GLN
3	C	287	ASN
3	C	323	GLN
3	C	325	GLN
3	C	342	ASN
3	C	463	HIS
3	C	549	ASN
3	C	607	GLN
3	C	648	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	13/15 (86%)	5 (38%)	1 (7%)
5	R	19/21 (90%)	3 (15%)	1 (5%)
6	V	13/14 (92%)	6 (46%)	1 (7%)
All	All	45/50 (90%)	14 (31%)	3 (6%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	2	A
4	M	5	G
4	M	6	C
4	M	8	A
4	M	9	U
5	R	11	C
5	R	14	C
5	R	15	U
6	V	5	G
6	V	6	U

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Mol	Chain	Res	Type
6	V	7	A
6	V	11	A
6	V	13	A
6	V	14	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	M	8	A
5	R	13	U
6	V	5	G

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 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
8	CTP	B	801	9	29,30,30	0.64	0	43,47,47	0.55	0
7	PO4	A	801	-	4,4,4	0.68	0	6,6,6	0.48	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
8	CTP	B	801	9	-	2/22/38/38	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

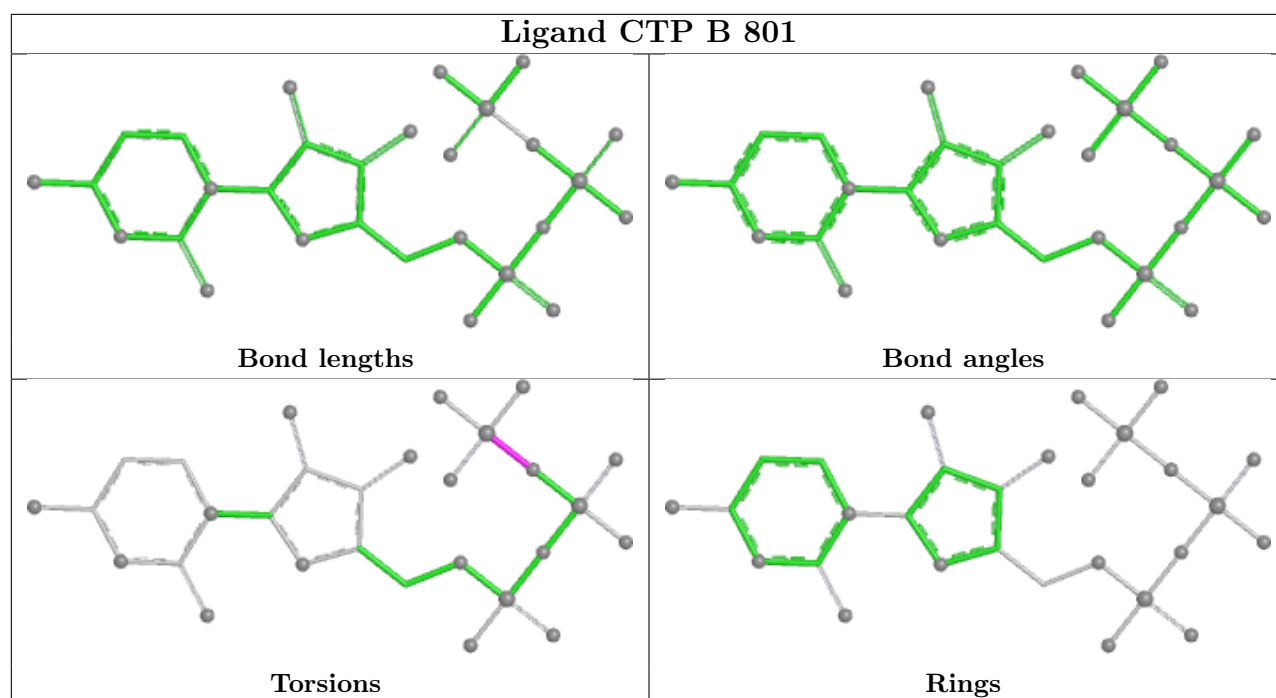
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	801	CTP	PB-O3B-PG-O2G
8	B	801	CTP	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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	717/751 (95%)	-0.09	13 (1%)	67 48	83, 117, 212, 228	0
2	B	746/772 (96%)	-0.08	12 (1%)	70 51	85, 113, 146, 180	0
3	C	733/798 (91%)	-0.03	12 (1%)	70 51	89, 123, 192, 238	0
4	M	14/15 (93%)	0.72	2 (14%)	6 5	124, 159, 197, 200	0
5	R	21/21 (100%)	-0.43	0	100 100	88, 102, 127, 139	0
6	V	14/14 (100%)	-0.97	0	100 100	88, 94, 100, 101	0
All	All	2245/2371 (94%)	-0.07	39 (1%)	69 49	83, 117, 199, 238	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	485	VAL	4.2
1	A	183	LEU	3.8
2	B	642	ALA	3.5
4	M	9	U	3.3
2	B	644	ILE	3.1
3	C	569	LYS	3.0
2	B	691	CYS	3.0
2	B	653	LYS	2.9
2	B	650	PRO	2.6
3	C	570	GLU	2.6
3	C	35	LYS	2.6
3	C	462	LEU	2.5
1	A	63	ALA	2.5
1	A	73	LEU	2.5
2	B	197	LYS	2.4
3	C	494	THR	2.4
1	A	546	VAL	2.4
1	A	138	LYS	2.4
2	B	678	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	651	VAL	2.3
1	A	71	GLN	2.3
3	C	207	TYR	2.2
1	A	189	VAL	2.1
2	B	633	HIS	2.1
3	C	385	LYS	2.1
2	B	125	GLY	2.1
1	A	723	ILE	2.1
1	A	83	MET	2.1
1	A	146	MET	2.1
3	C	516	ALA	2.1
2	B	473	GLY	2.1
1	A	125	LYS	2.1
3	C	43	LYS	2.1
1	A	195	ASP	2.1
4	M	6	C	2.1
3	C	480	VAL	2.0
3	C	342	ASN	2.0
2	B	652	LYS	2.0
1	A	297	GLY	2.0

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](#)

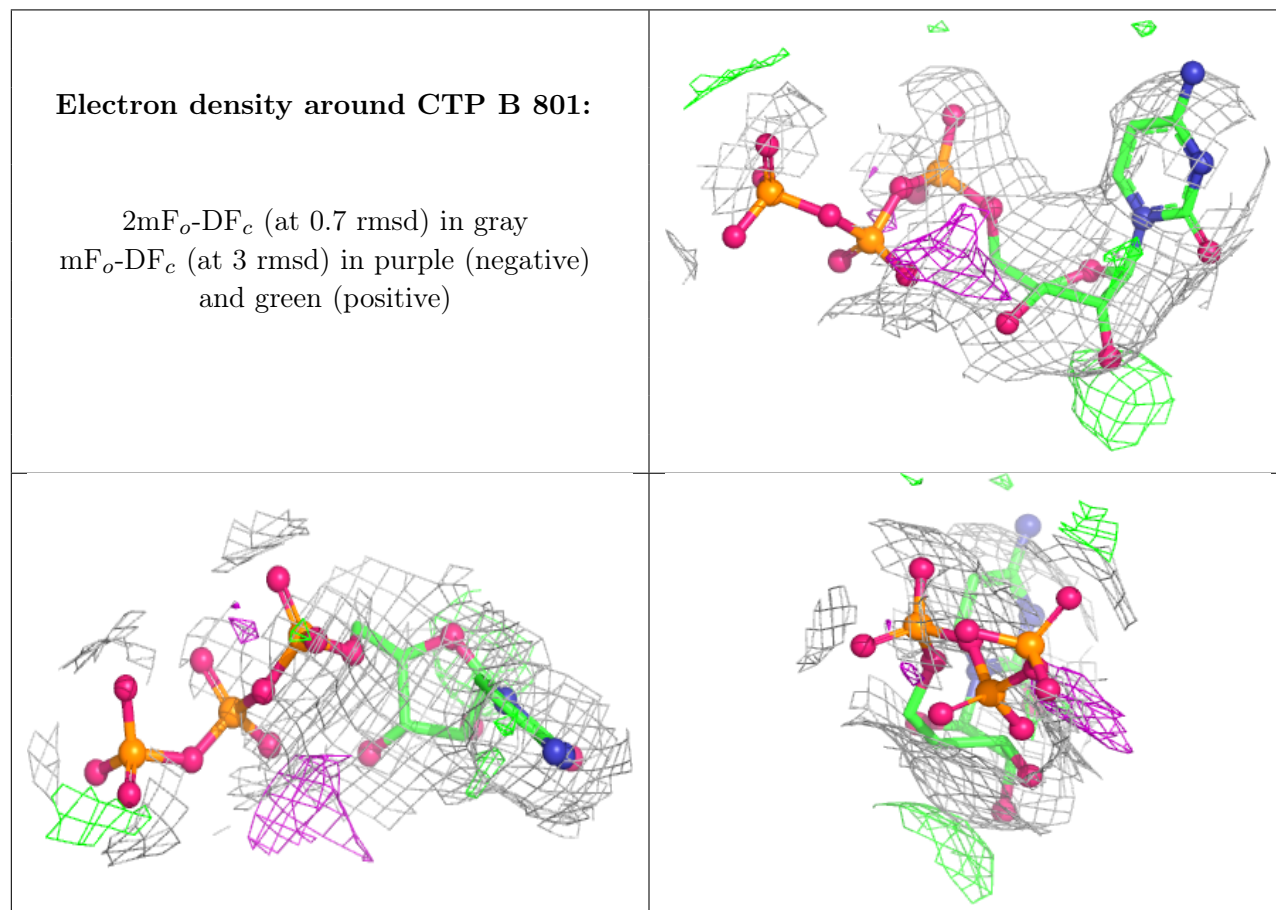
There are no oligosaccharides in this entry.

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
7	PO4	A	801	5/5	0.85	0.12	139,140,141,141	0
8	CTP	B	801	29/29	0.93	0.10	121,135,146,152	0
9	MG	B	802	1/1	0.97	0.07	129,129,129,129	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 ⓘ

There are no such residues in this entry.