



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:58 PM UTC

PDB ID : 3CFR / pdb_00003cfr
Title : Structure of the replicating complex of a POL Alpha family DNA Polymerase, ternary complex 2
Authors : Wang, J.; Klimenko, D.; Wang, M.; Steitz, T.A.; Konigsberg, W.H.
Deposited on : 2008-03-04
Resolution : 2.40 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

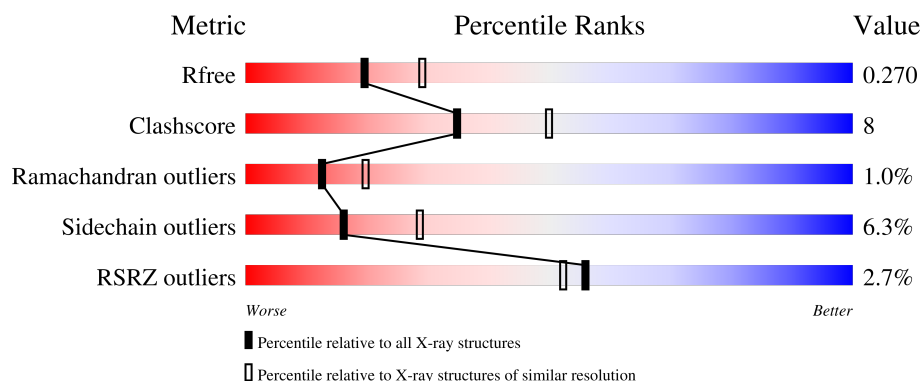
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	18	6% 72% 22% 6%
2	P	13	77% 15% 8%
3	A	909	3% 80% 16% ...

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (5'-D(*DTP*DCP*DAP*DAP*DGP*DTP*DAP*DAP*DGP*DCP*DAP*DGP*DTP*DCP*DCP*DGP*DCP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	18	Total	C	N	O	P	0	0	0
			367	175	71	104	17			

- Molecule 2 is a DNA chain called DNA (5'-D(*DGP*DCP*DGP*DGP*DAP*DCP*DTP*DGP*DCP*DTP*DTP*DAP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	901	Total	C	N	O	S	0	0	0
			7343	4714	1224	1372	33			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ALA	LEU	engineered mutation	UNP Q38087
A	565	GLY	SER	engineered mutation	UNP Q38087
A	567	ALA	TYR	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
A	907	HIS	-	expression tag	UNP Q38087
A	908	HIS	-	expression tag	UNP Q38087
A	909	HIS	-	expression tag	UNP Q38087

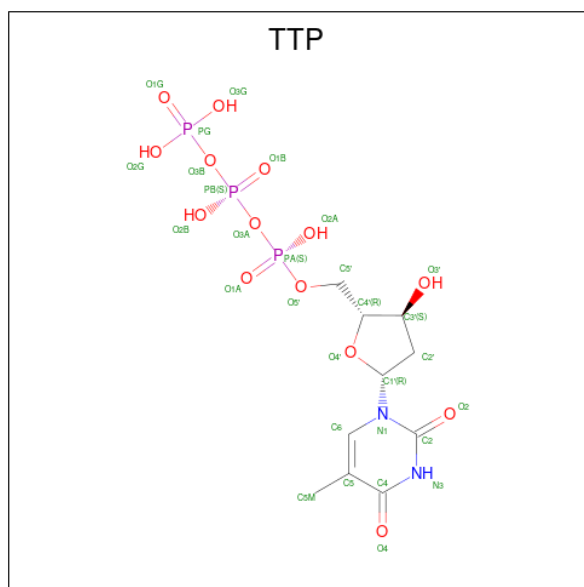
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 29 10 2 14 3	0	0

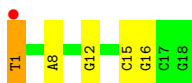
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	30	Total O 30 30	0	0
7	P	16	Total O 16 16	0	0
7	A	583	Total O 583 583	0	0

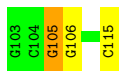
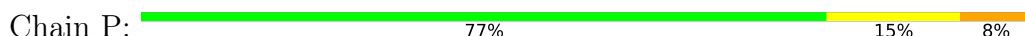
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

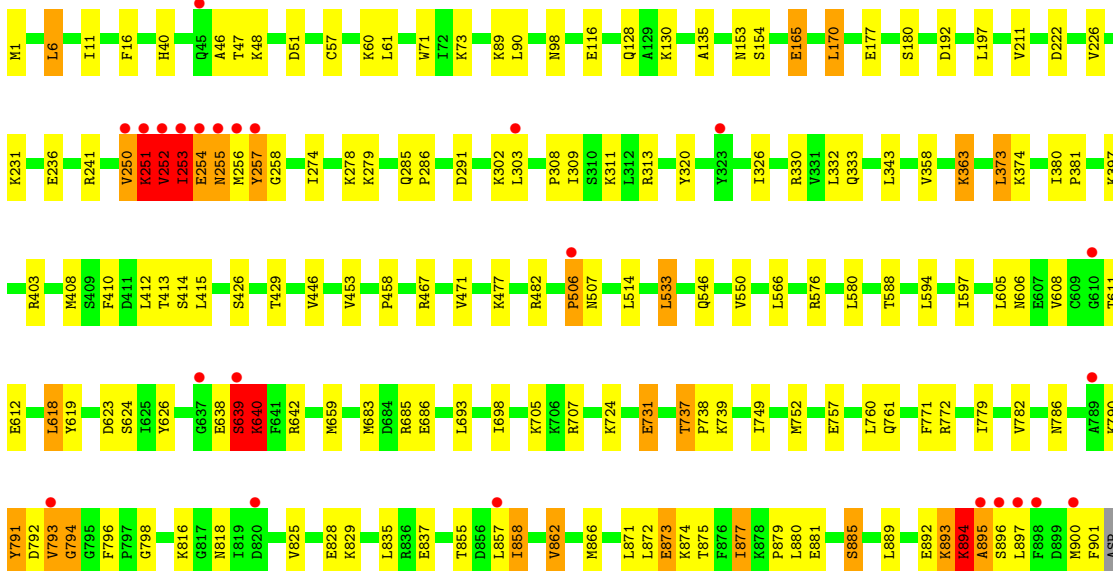
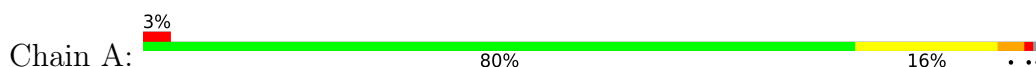
- Molecule 1: DNA (5'-D(*DTP*DCP*DAP*DAP*DGP*DTP*DAP*DAP*DGP*DCP*DAP*DG*P*DTP*DCP*DCP*DCP*DG)-3')



- Molecule 2: DNA (5'-D(*DGP*DCP*DGP*DGP*DAP*DCP*DTP*DGP*DCP*DTP*DTP*DA*P*(DOC))-3')



- Molecule 3: DNA polymerase



PHE
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.96Å 119.77Å 130.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.40) 99.6 (50.00-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.266 0.202 , 0.270	Depositor DCC
R_{free} test set	2340 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8636	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, TTP, DOC, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	T	0.30	0/412	1.07	2/634 (0.3%)
2	P	0.30	0/273	1.02	1/420 (0.2%)
3	A	0.54	0/7522	0.90	14/10164 (0.1%)
All	All	0.53	0/8207	0.91	17/11218 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	791	TYR	N-CA-C	9.72	128.49	114.39
3	A	791	TYR	CA-C-N	6.88	134.09	121.70
3	A	791	TYR	C-N-CA	6.88	134.09	121.70
3	A	639	SER	CA-C-N	6.59	133.57	121.70
3	A	639	SER	C-N-CA	6.59	133.57	121.70
2	P	105	DG	P-O3'-C3'	6.26	129.59	120.20
1	T	1	DT	C1'-O4'-C4'	-5.82	100.97	109.70
3	A	250	VAL	CA-C-N	5.39	131.40	121.70
3	A	250	VAL	C-N-CA	5.39	131.40	121.70
3	A	877	ILE	N-CA-C	5.37	115.58	110.42
3	A	893	LYS	CA-C-N	5.31	131.26	121.70
3	A	893	LYS	C-N-CA	5.31	131.26	121.70
1	T	1	DT	P-O3'-C3'	5.27	128.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	251	LYS	CA-C-N	5.24	131.13	121.70
3	A	251	LYS	C-N-CA	5.24	131.13	121.70
3	A	252	VAL	CA-C-N	5.07	130.83	121.70
3	A	252	VAL	C-N-CA	5.07	130.83	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	506	PRO	Peptide
3	A	792	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	367	0	203	5	0
2	P	262	0	148	2	0
3	A	7343	0	7236	114	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	29	0	13	0	0
7	A	583	0	0	16	0
7	P	16	0	0	0	0
7	T	30	0	0	0	0
All	All	8636	0	7600	117	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 (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:639:SER:HB2	3:A:640:LYS:HB2	1.16	1.09
3:A:895:ALA:HB3	3:A:896:SER:HA	1.29	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:895:ALA:CB	3:A:896:SER:HA	1.80	1.05
3:A:254:GLU:CB	3:A:255:ASN:HA	1.90	1.01
3:A:254:GLU:HB3	3:A:255:ASN:HA	1.03	1.01
3:A:254:GLU:HB3	3:A:255:ASN:CA	1.94	0.95
3:A:639:SER:CB	3:A:640:LYS:HB2	1.95	0.95
3:A:506:PRO:HA	3:A:507:ASN:HB2	1.53	0.88
1:T:1:DT:H3	3:A:786:ASN:ND2	1.84	0.75
3:A:257:TYR:N	3:A:257:TYR:HD2	1.86	0.73
3:A:170:LEU:HA	3:A:177:GLU:HG3	1.72	0.72
3:A:291:ASP:HB2	7:A:1191:HOH:O	1.88	0.72
3:A:896:SER:N	3:A:897:LEU:HA	2.04	0.72
3:A:900:MET:HA	3:A:901:PHE:C	2.15	0.70
3:A:257:TYR:N	3:A:257:TYR:CD2	2.59	0.69
3:A:222:ASP:O	3:A:226:VAL:HG12	1.95	0.66
3:A:252:VAL:H	3:A:253:ILE:HG22	1.60	0.66
3:A:825:VAL:HB	3:A:828:GLU:HG3	1.78	0.65
3:A:477:LYS:HD3	7:A:1382:HOH:O	1.96	0.65
3:A:313:ARG:NH1	7:A:1132:HOH:O	2.13	0.64
3:A:250:VAL:HA	3:A:251:LYS:HB2	1.79	0.64
3:A:330:ARG:HH11	3:A:333:GLN:HE22	1.43	0.63
3:A:857:LEU:O	3:A:858:ILE:HG12	1.99	0.62
3:A:685:ARG:HD3	7:A:1403:HOH:O	2.00	0.62
3:A:252:VAL:N	3:A:253:ILE:HG22	2.15	0.61
3:A:892:GLU:O	3:A:894:LYS:HB3	2.01	0.61
3:A:794:GLY:H	3:A:796:PHE:H	1.50	0.59
3:A:274:ILE:HG12	3:A:278:LYS:HE3	1.85	0.58
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.86	0.58
3:A:873:GLU:HA	3:A:877:ILE:HB	1.86	0.57
3:A:896:SER:H	3:A:897:LEU:HA	1.68	0.57
3:A:791:TYR:O	3:A:798:GLY:N	2.20	0.57
3:A:618:LEU:HD13	3:A:626:TYR:O	2.06	0.56
1:T:1:DT:H3	3:A:786:ASN:HD21	1.51	0.56
3:A:731:GLU:HG3	3:A:879:PRO:HB3	1.88	0.56
3:A:779:ILE:HD11	3:A:866:MET:HE1	1.87	0.56
3:A:40:HIS:HE1	3:A:51:ASP:OD2	1.89	0.55
3:A:546:GLN:O	3:A:550:VAL:HG23	2.07	0.55
3:A:639:SER:CA	3:A:640:LYS:HB2	2.37	0.54
3:A:893:LYS:HA	3:A:894:LYS:CB	2.38	0.54
3:A:241:ARG:NH2	7:A:1193:HOH:O	2.41	0.54
3:A:47:THR:HG21	3:A:57:CYS:O	2.08	0.53
3:A:900:MET:CA	3:A:901:PHE:C	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:373:LEU:HD23	3:A:380:ILE:HG22	1.91	0.53
3:A:737:THR:HG22	7:A:1122:HOH:O	2.08	0.52
1:T:15:DC:H2"	1:T:16:DG:C8	2.44	0.52
3:A:790:LYS:O	3:A:790:LYS:HG2	2.09	0.52
3:A:90:LEU:HD11	3:A:363:LYS:HE2	1.90	0.51
3:A:707:ARG:HH22	3:A:731:GLU:CD	2.19	0.51
3:A:286:PRO:HB3	3:A:782:VAL:HG21	1.92	0.51
3:A:412:LEU:HD13	3:A:415:LEU:HD13	1.93	0.51
3:A:858:ILE:O	3:A:862:VAL:HG13	2.11	0.51
3:A:308:PRO:HG2	3:A:311:LYS:HG3	1.94	0.50
3:A:330:ARG:HH11	3:A:333:GLN:NE2	2.11	0.49
3:A:1:MET:HA	7:A:1192:HOH:O	2.13	0.49
3:A:893:LYS:HA	3:A:894:LYS:CG	2.43	0.49
3:A:251:LYS:HA	3:A:252:VAL:O	2.13	0.48
3:A:408:MET:CE	3:A:659:MET:HE1	2.42	0.48
3:A:255:ASN:ND2	3:A:255:ASN:H	2.11	0.48
3:A:60:LYS:HD2	3:A:71:TRP:CZ2	2.49	0.48
1:T:8:DA:H5"	3:A:705:LYS:HD3	1.94	0.48
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.96	0.48
3:A:255:ASN:ND2	3:A:256:MET:H	2.11	0.48
2:P:105:DG:H2"	2:P:106:DG:H8	1.79	0.48
3:A:250:VAL:CA	3:A:251:LYS:HB2	2.42	0.47
3:A:330:ARG:NH1	3:A:333:GLN:HE22	2.12	0.47
3:A:895:ALA:CB	3:A:896:SER:CA	2.70	0.47
3:A:779:ILE:HB	3:A:871:LEU:HD21	1.95	0.47
3:A:426:SER:HB3	3:A:429:THR:OG1	2.14	0.46
3:A:771:PHE:CE1	3:A:872:LEU:HD22	2.50	0.46
3:A:467:ARG:HG3	7:A:1445:HOH:O	2.15	0.46
3:A:153:ASN:HB2	3:A:192:ASP:O	2.16	0.46
3:A:724:LYS:HD3	7:A:1295:HOH:O	2.15	0.46
3:A:640:LYS:HD2	7:A:1296:HOH:O	2.15	0.45
3:A:458:PRO:HG2	3:A:588:THR:HG22	1.97	0.45
3:A:749:ILE:HA	3:A:752:MET:HE3	1.97	0.45
3:A:471:VAL:HG13	3:A:566:LEU:HD21	1.98	0.45
3:A:130:LYS:HB3	7:A:1453:HOH:O	2.16	0.45
3:A:514:LEU:HD13	3:A:533:LEU:HD21	1.98	0.45
3:A:597:ILE:HD12	3:A:597:ILE:HA	1.92	0.45
3:A:605:LEU:HA	3:A:608:VAL:HG12	2.00	0.44
3:A:862:VAL:O	3:A:866:MET:HG3	2.17	0.44
1:T:12:DG:OP1	3:A:874:LYS:HE3	2.18	0.44
3:A:231:LYS:HG3	3:A:236:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:410:PHE:HB3	3:A:683:MET:HG2	2.01	0.43
3:A:881:GLU:O	3:A:885:SER:HB3	2.18	0.43
3:A:731:GLU:CG	3:A:879:PRO:HB3	2.47	0.43
3:A:772:ARG:HG3	7:A:1340:HOH:O	2.19	0.43
3:A:793:VAL:O	3:A:796:PHE:O	2.37	0.43
3:A:397:LYS:HD3	3:A:619:TYR:HA	2.00	0.43
3:A:738:PRO:HB3	3:A:779:ILE:HA	2.00	0.42
3:A:415:LEU:HD22	3:A:623:ASP:CB	2.48	0.42
3:A:256:MET:HA	3:A:257:TYR:HA	1.76	0.42
3:A:413:THR:O	3:A:414:SER:C	2.62	0.42
3:A:606:ASN:OD1	3:A:611:THR:HG23	2.18	0.42
3:A:698:ILE:HG21	3:A:889:LEU:HD11	2.01	0.42
3:A:381:PRO:O	3:A:576:ARG:HD3	2.19	0.42
3:A:255:ASN:HD22	3:A:256:MET:N	2.17	0.42
3:A:165:GLU:H	3:A:165:GLU:CD	2.28	0.42
3:A:893:LYS:HA	3:A:894:LYS:HB3	2.01	0.42
3:A:313:ARG:HG3	3:A:320:TYR:CD2	2.55	0.42
3:A:403:ARG:NH2	3:A:889:LEU:HD12	2.35	0.42
3:A:257:TYR:HA	3:A:258:GLY:HA2	1.86	0.41
3:A:6:LEU:HG	3:A:211:VAL:HG21	2.02	0.41
3:A:11:ILE:HD12	3:A:16:PHE:CD2	2.55	0.41
3:A:128:GLN:HG3	7:A:1473:HOH:O	2.21	0.41
3:A:46:ALA:HB3	7:A:1485:HOH:O	2.20	0.41
3:A:482:ARG:C	3:A:482:ARG:HD3	2.46	0.41
3:A:875:THR:O	3:A:879:PRO:HG2	2.20	0.41
3:A:893:LYS:HA	3:A:894:LYS:HG2	2.02	0.41
3:A:285:GLN:O	3:A:829:LYS:NZ	2.50	0.41
3:A:757:GLU:O	3:A:761:GLN:HG3	2.21	0.41
3:A:326:ILE:O	3:A:330:ARG:HG2	2.21	0.40
3:A:279:LYS:HE2	3:A:358:VAL:O	2.20	0.40
3:A:51:ASP:HB2	7:A:1196:HOH:O	2.20	0.40
3:A:89:LYS:HG3	7:A:1057:HOH:O	2.20	0.40
2:P:105:DG:H2"	2:P:106:DG:C8	2.55	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	
3	A	899/909 (99%)	859 (96%)	31 (3%)	9 (1%)	12	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	858	ILE
3	A	251	LYS
3	A	640	LYS
3	A	895	ALA
3	A	639	SER
3	A	252	VAL
3	A	253	ILE
3	A	794	GLY
3	A	894	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	795/805 (99%)	745 (94%)	50 (6%)	16	29

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	LEU
3	A	48	LYS

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Mol	Chain	Res	Type
3	A	61	LEU
3	A	73	LYS
3	A	98	ASN
3	A	154	SER
3	A	165	GLU
3	A	170	LEU
3	A	180	SER
3	A	197	LEU
3	A	253	ILE
3	A	254	GLU
3	A	255	ASN
3	A	257	TYR
3	A	302	LYS
3	A	303	LEU
3	A	309	ILE
3	A	332	LEU
3	A	343	LEU
3	A	363	LYS
3	A	373	LEU
3	A	374	LYS
3	A	446	VAL
3	A	453	VAL
3	A	533	LEU
3	A	580	LEU
3	A	594	LEU
3	A	612	GLU
3	A	618	LEU
3	A	624	SER
3	A	638	GLU
3	A	640	LYS
3	A	642	ARG
3	A	686	GLU
3	A	693	LEU
3	A	731	GLU
3	A	737	THR
3	A	739	LYS
3	A	760	LEU
3	A	793	VAL
3	A	816	LYS
3	A	818	ASN
3	A	835	LEU
3	A	837	GLU

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Mol	Chain	Res	Type
3	A	855	THR
3	A	862	VAL
3	A	873	GLU
3	A	880	LEU
3	A	885	SER
3	A	894	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	98	ASN
3	A	105	HIS
3	A	131	HIS
3	A	153	ASN
3	A	203	ASN
3	A	255	ASN
3	A	333	GLN
3	A	339	GLN
3	A	354	GLN
3	A	539	ASN
3	A	546	GLN
3	A	564	ASN
3	A	678	GLN
3	A	761	GLN
3	A	786	ASN
3	A	823	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	115	1,2	16,19,20	0.92	1 (6%)	20,26,29	1.27	3 (15%)

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	115	1,2	-	2/7/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	115	DOC	C6-C5	2.15	1.40	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	115	DOC	O4'-C1'-N1	2.90	113.01	107.86
2	P	115	DOC	C3'-C2'-C1'	2.76	106.05	102.87
2	P	115	DOC	O4'-C4'-C3'	2.22	108.46	104.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	115	DOC	O4'-C4'-C5'-O5'
2	P	115	DOC	C3'-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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TTP	A	916	4	29,30,30	1.36	5 (17%)	43,47,47	1.86	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TTP	A	916	4	-	2/22/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	916	TTP	PB-O3A	3.10	1.62	1.59
6	A	916	TTP	C6-C5	3.03	1.39	1.34
6	A	916	TTP	C4-C5	2.69	1.49	1.44
6	A	916	TTP	C4-N3	-2.25	1.34	1.38
6	A	916	TTP	PA-O3A	2.14	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	916	TTP	N3-C2-N1	5.08	121.51	114.89
6	A	916	TTP	C4-N3-C2	-4.86	120.97	127.34
6	A	916	TTP	C5-C4-N3	4.00	118.80	115.32
6	A	916	TTP	O4-C4-C5	-3.94	120.41	124.92
6	A	916	TTP	O2-C2-N1	-3.63	118.07	122.80
6	A	916	TTP	O4'-C1'-N1	3.09	113.34	107.86
6	A	916	TTP	O2B-PB-O3A	3.00	115.38	107.27
6	A	916	TTP	C5-C6-N1	-2.79	120.28	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	916	TTP	C2'-C1'-N1	-2.42	107.77	113.81
6	A	916	TTP	C5M-C5-C4	2.22	121.15	118.78

There are no chirality outliers.

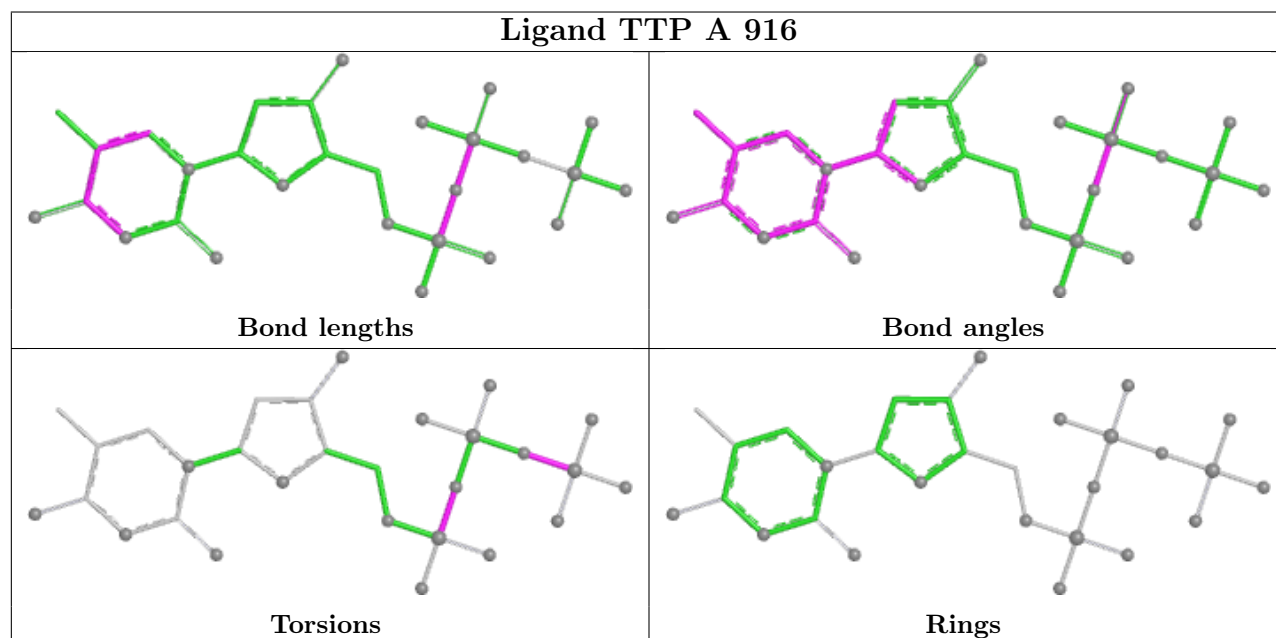
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	916	TTP	PB-O3A-PA-O5'
6	A	916	TTP	PB-O3B-PG-O2G

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	T	18/18 (100%)	-0.54	1 (5%) 30 26	14, 22, 44, 65	0
2	P	12/13 (92%)	-0.28	0 100 100	18, 29, 46, 52	0
3	A	901/909 (99%)	-0.16	24 (2%) 56 52	17, 29, 49, 80	0
All	All	931/940 (99%)	-0.17	25 (2%) 56 52	14, 29, 49, 80	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	257	TYR	6.4
3	A	253	ILE	4.3
3	A	250	VAL	4.0
3	A	255	ASN	3.9
3	A	857	LEU	3.6
3	A	252	VAL	3.5
3	A	793	VAL	3.2
3	A	789	ALA	3.2
3	A	256	MET	3.1
3	A	898	PHE	3.0
1	T	1	DT	3.0
3	A	897	LEU	2.9
3	A	506	PRO	2.9
3	A	900	MET	2.8
3	A	896	SER	2.8
3	A	895	ALA	2.8
3	A	639	SER	2.8
3	A	254	GLU	2.8
3	A	637	GLY	2.2
3	A	251	LYS	2.2
3	A	820	ASP	2.2
3	A	323	TYR	2.1
3	A	303	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	610	GLY	2.0
3	A	45	GLN	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	115	18/19	0.96	0.06	16,18,20,21	0

6.3 Carbohydrates [i](#)

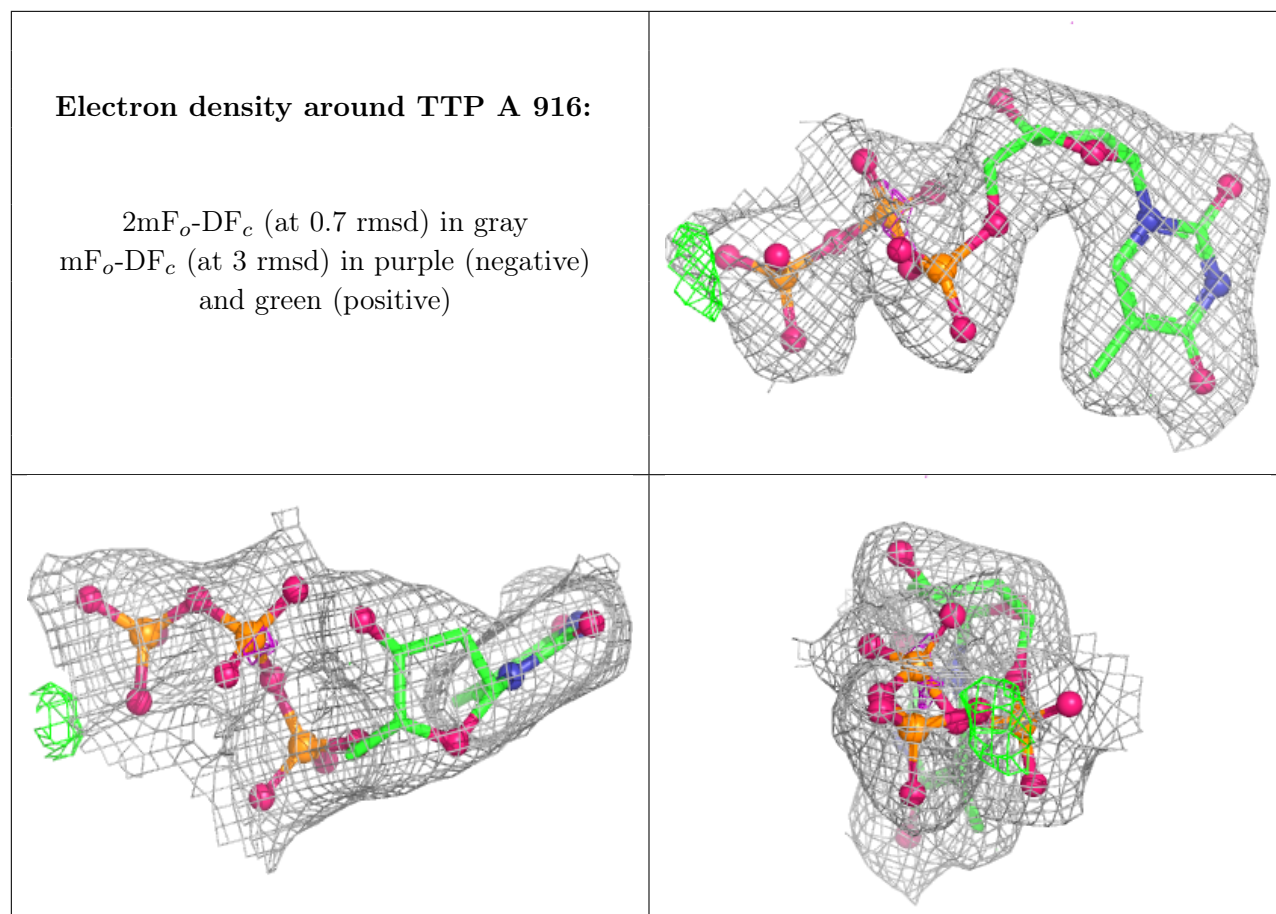
There are no oligosaccharides in this entry.

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
4	CA	A	912	1/1	0.76	0.32	91,91,91,91	0
4	CA	A	914	1/1	0.88	0.13	61,61,61,61	0
5	CL	A	915	1/1	0.94	0.09	55,55,55,55	0
4	CA	A	911	1/1	0.95	0.06	57,57,57,57	0
6	TTP	A	916	29/29	0.95	0.07	17,22,31,32	0
4	CA	A	913	1/1	0.96	0.11	48,48,48,48	0
4	CA	A	910	1/1	0.96	0.08	48,48,48,48	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.