



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 01:20 AM UTC

PDB ID : 3CQ8 / pdb_00003cq8
Title : Ternary complex of the L415F mutant RB69 exo(-)polymerase
Authors : Zhong, X.; Pedersen, L.C.; Kunkel, T.A.
Deposited on : 2008-04-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

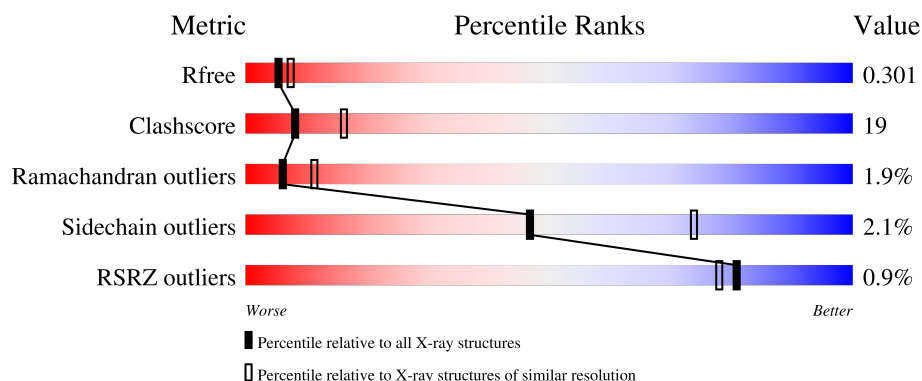
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

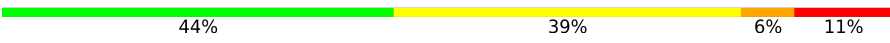
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
2	P	14	
3	A	903	

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
7	GOL	A	1100	-	X	-	-
7	GOL	A	1101	-	X	-	-
7	GOL	A	1102	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8484 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(*DAP*DCP*DAP*DGP*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
			369	175	74	103	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			281	135	51	82	13			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	902	Total	C	N	O	S	0	0	0
			7345	4720	1219	1373	33			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	415	PHE	LEU	engineered mutation	UNP Q38087

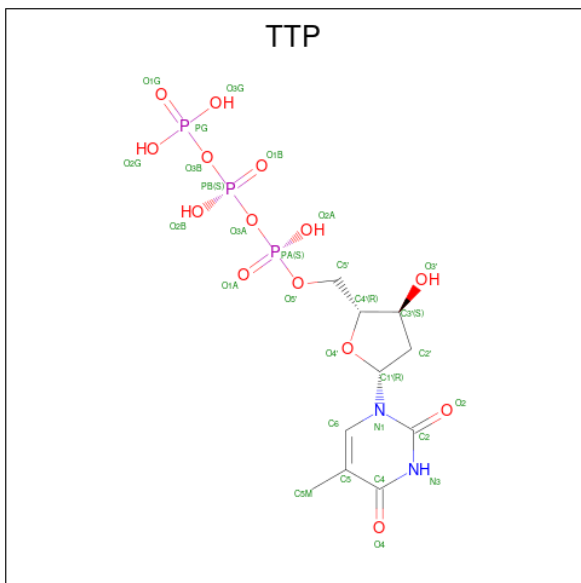
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Ca	0	0
			6	6		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

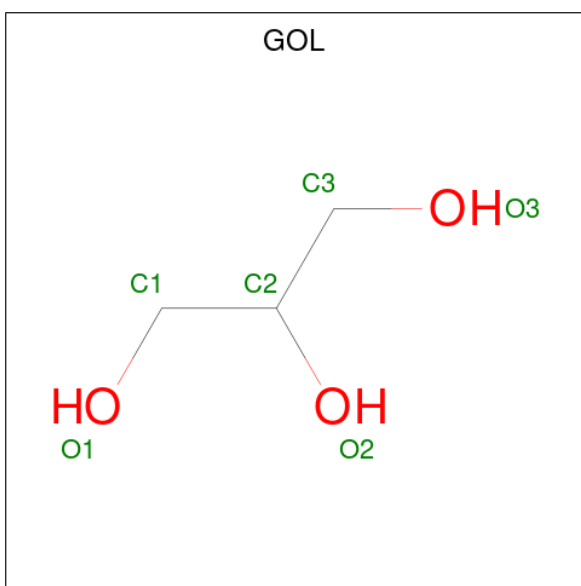
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Na 3 3	0	0

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_2\text{O}_{14}\text{P}_3$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

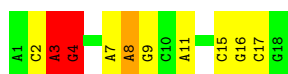


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

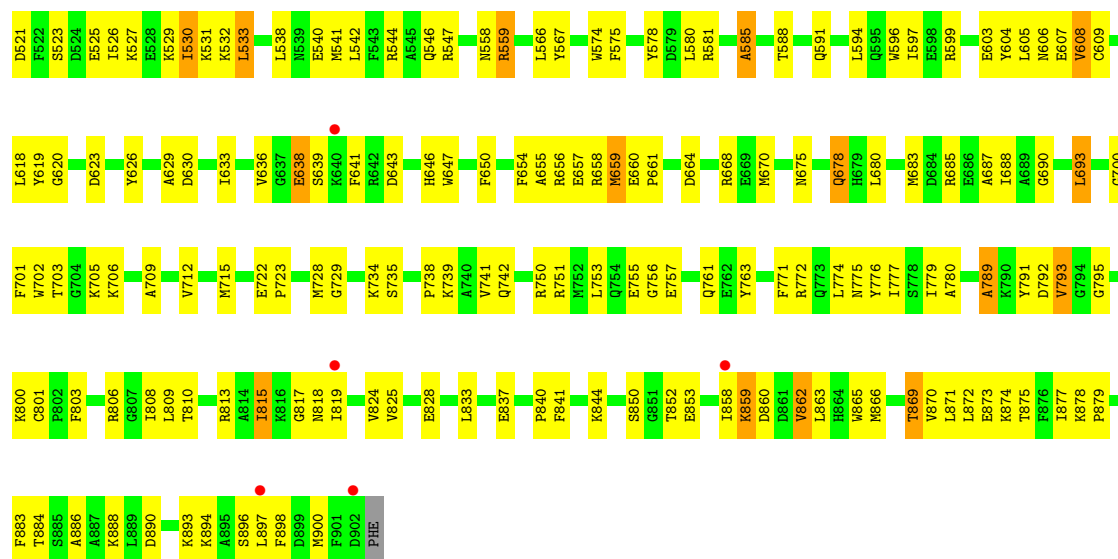
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	T	28	Total	O	0	0
			28	28		
8	P	16	Total	O	0	0
			16	16		
8	A	389	Total	O	0	0
			389	389		

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



T433	Q339	Y217	Ti15	M1
V436	N342	S220	Ei16	K2
A437		F221		E3
P438		A222	D121	T7
	A351	I223		
D441	K352	P224	P124	D13
	I353	Y225		S14
R449	Q354	V226	Q128	I15
P450	I355		A129	
S451	Q356	R229	K130	R18
D452	S357	I230	Y19	K18
V453	V358	K231	H131	Y19
Y454	S360		P132	I20
S455	F369	F234	I136	D21
C456	P361	G235	T137	S22
S457	I362	E236		N23
P458		S937	D150	G24
M459	F370	T238	L151	R25
G460			L152	E26
M461	K373	R246	N153	Y33
M462	L374			K34
Y463	E375	E254	M158	S35
Y464	Q376	N255	V159	S36
K465	N377	M256		L37
D466	K378	Y257	S163	F38
R467	V379	G258	I164	A39
D468	I380	E165	E166	H40
G469	P381	R260		
V470	Q382			E43
P471		I263	K169	S44
P472	Q389		L170	
Q431	F395	I274	Q171	K48
	V396	D275	E172	Y49
	G397		Q173	
L490	E398	K279	E177	K55
		F280		P56
R494	P401	N284	I186	F62
N495	M402	Q285		A63
G496			P190	N64
I499	K405	K302	F191	M65
K500	Y406	L303	D192	R66
E501	V407	K304	N193	D67
A502	M408	Y305	E194	A68
L503		D306	K195	
H504	D411		E196	I72
H505	L412	I309	L197	
P506	T413		L198	A82
N507	S414	R313	M199	L83
L508	F415	E314	E200	G84
S509		S315	Y201	M85
V510	R421	N316		
	Q422	H317	F204	L90
D511				
E512	S426	I325	P210	S94
L514	P427		V211	
	E428	Y329		K107
Y518	T429		G215	
		Q232	Y216	A111



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.84Å 117.01Å 127.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.70 – 2.50 25.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	79.8 (25.70-2.50) 79.7 (25.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.281 0.231 , 0.301	Depositor DCC
R_{free} test set	2110 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8484	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: GOL, TTP, CA, NA

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	0.31	0/415	0.81	2/639 (0.3%)
2	P	0.33	0/314	0.61	0/482
3	A	0.44	0/7526	0.93	26/10174 (0.3%)
All	All	0.43	0/8255	0.91	28/11295 (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
1	T	0	3
2	P	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	VAL	N-CA-C	-11.07	101.15	111.67
1	T	3	DA	N9-C1'-C2'	-7.11	102.83	113.50
3	A	559	ARG	N-CA-C	-6.97	103.45	112.23
3	A	606	ASN	N-CA-C	-6.95	104.83	113.38
3	A	566	LEU	N-CA-C	-6.78	103.97	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	112	DT	Sidechain
1	T	3	DA	Sidechain
1	T	4	DG	Sidechain
1	T	8	DA	Sidechain

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	369	0	202	14	0
2	P	281	0	157	9	0
3	A	7345	0	7213	291	0
4	A	6	0	0	0	0
5	A	3	0	0	0	0
6	A	29	0	13	0	0
7	A	18	0	18	2	0
8	A	389	0	0	19	0
8	P	16	0	0	0	0
8	T	28	0	0	0	0
All	All	8484	0	7603	304	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 19.

The worst 5 of 304 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:712:VAL:HG11	3:A:715:MET:HE2	1.45	0.95
3:A:373:LEU:HD21	3:A:470:VAL:HG21	1.53	0.91
3:A:428:GLU:OE2	3:A:470:VAL:HG23	1.71	0.89
2:P:114:DC:H2"	2:P:115:DC:H5"	1.54	0.89
3:A:481:GLN:HB3	3:A:559:ARG:HD3	1.59	0.83

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	900/903 (100%)	793 (88%)	90 (10%)	17 (2%)	6 11

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	121	ASP
3	A	608	VAL
3	A	818	ASN
3	A	306	ASP
3	A	402	ASN

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	793/800 (99%)	776 (98%)	17 (2%)	47 74

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	678	GLN
3	A	869	THR
3	A	406	TYR
3	A	436	VAL
3	A	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	389	GLN
3	A	493	GLN
3	A	864	HIS
3	A	761	GLN
3	A	158	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z > 2$
7	GOL	A	1100	-	5,5,5	2.99	1 (20%)	5,5,5	2.46	4 (80%)
6	TTP	A	1010	4	29,30,30	1.97	7 (24%)	43,47,47	1.27	4 (9%)
7	GOL	A	1101	-	5,5,5	3.12	1 (20%)	5,5,5	2.36	4 (80%)
7	GOL	A	1102	-	5,5,5	3.02	1 (20%)	5,5,5	2.30	2 (40%)

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
7	GOL	A	1100	-	-	2/4/4/4	-
6	TTP	A	1010	4	-	3/22/34/34	0/2/2/2
7	GOL	A	1101	-	-	2/4/4/4	-
7	GOL	A	1102	-	-	3/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1101	GOL	O2-C2	-6.98	1.23	1.43
7	A	1102	GOL	O2-C2	-6.76	1.23	1.43
7	A	1100	GOL	O2-C2	-6.68	1.24	1.43
6	A	1010	TTP	PA-O3A	-5.55	1.53	1.59
6	A	1010	TTP	PG-O1G	-3.60	1.39	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1010	TTP	C6-C5-C4	-3.06	115.50	118.02
6	A	1010	TTP	O4'-C1'-N1	2.94	113.08	107.86
7	A	1101	GOL	O2-C2-C1	2.85	120.98	109.18
7	A	1100	GOL	O2-C2-C3	2.84	120.93	109.18
7	A	1102	GOL	O2-C2-C1	2.83	120.88	109.18

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1100	GOL	O1-C1-C2-C3
7	A	1101	GOL	O1-C1-C2-C3
7	A	1101	GOL	C1-C2-C3-O3
7	A	1100	GOL	O2-C2-C3-O3
7	A	1102	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

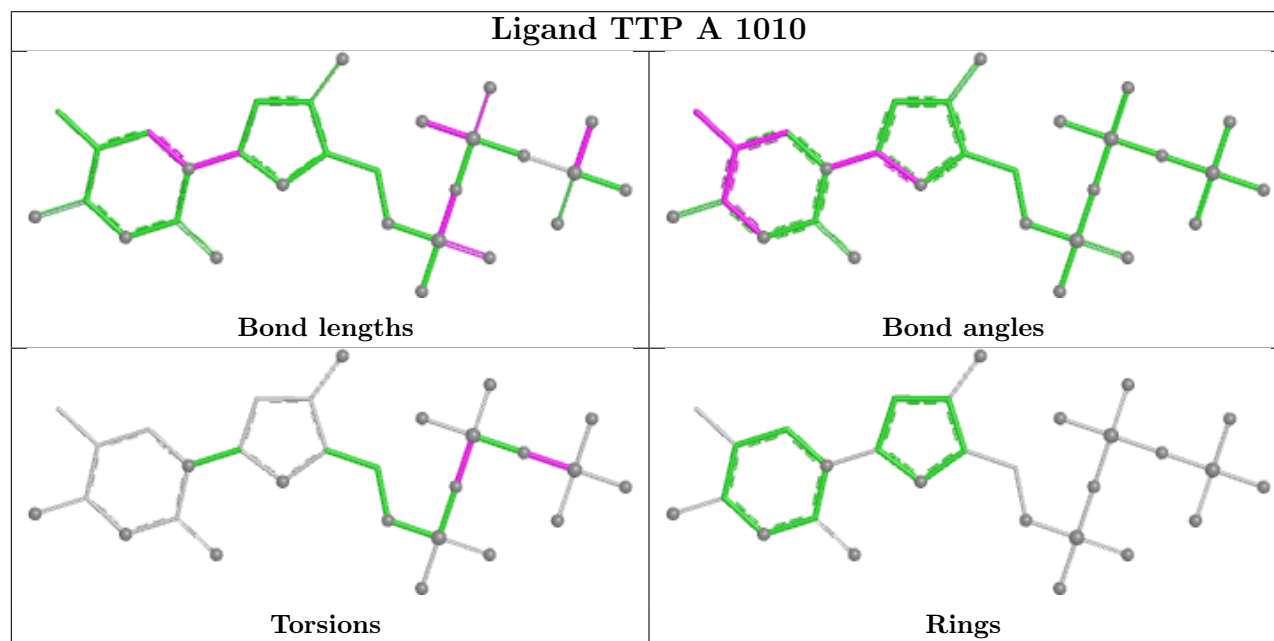
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1100	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1101	GOL	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.43	0	100	100	28, 43, 79, 106	0
2	P	14/14 (100%)	-0.23	0	100	100	27, 45, 76, 82	0
3	A	902/903 (99%)	-0.08	8 (0%)	81	78	22, 45, 77, 103	0
All	All	934/935 (99%)	-0.09	8 (0%)	81	78	22, 45, 77, 106	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	858	ILE	3.0
3	A	897	LEU	2.7
3	A	510	VAL	2.7
3	A	640	LYS	2.6
3	A	902	ASP	2.5

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](#)

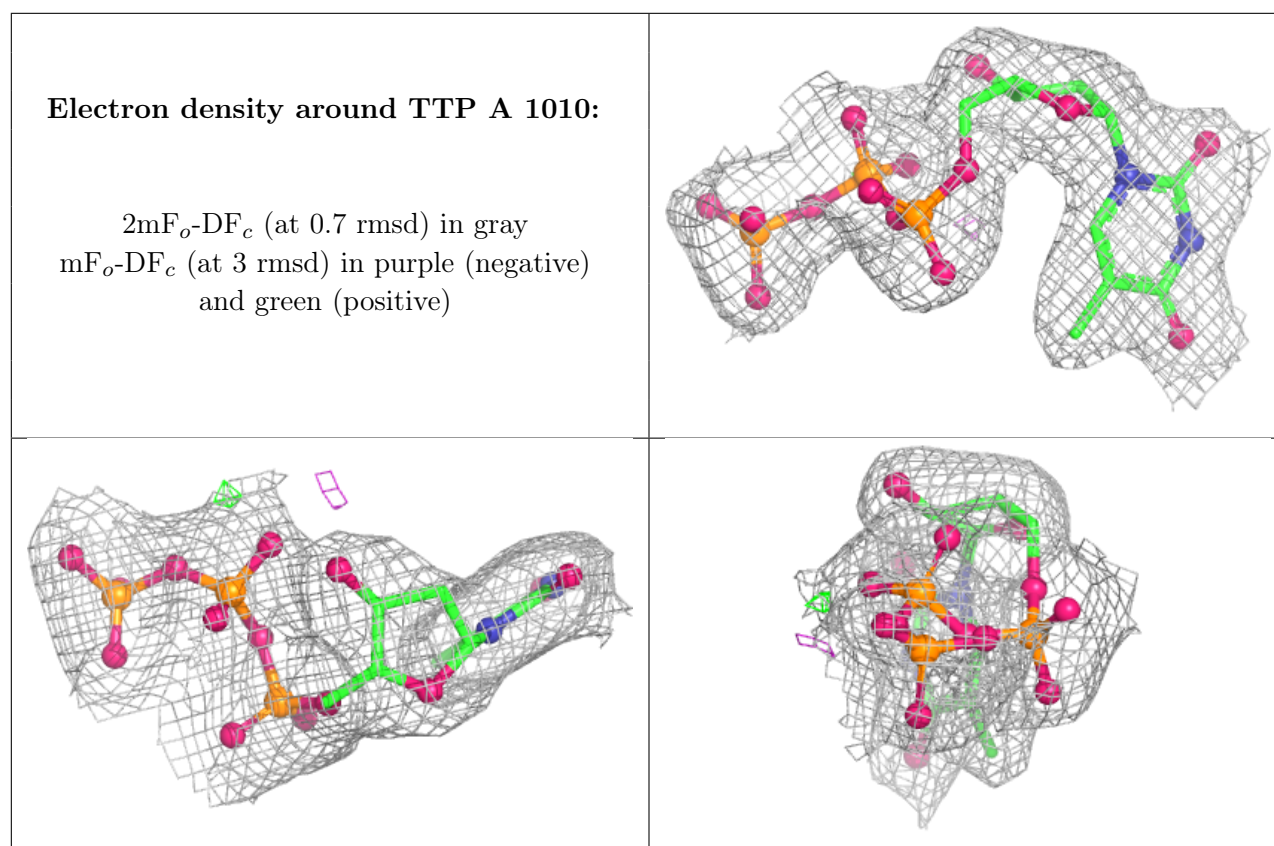
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
5	NA	A	1007	1/1	0.78	0.14	45,45,45,45	0
4	CA	A	1002	1/1	0.83	0.10	87,87,87,87	0
4	CA	A	1006	1/1	0.88	0.07	70,70,70,70	0
5	NA	A	1008	1/1	0.89	0.13	67,67,67,67	0
7	GOL	A	1100	6/6	0.89	0.10	39,45,46,46	0
7	GOL	A	1102	6/6	0.90	0.09	41,49,50,51	0
7	GOL	A	1101	6/6	0.93	0.08	43,44,45,45	0
5	NA	A	1009	1/1	0.94	0.08	56,56,56,56	0
4	CA	A	1005	1/1	0.94	0.05	72,72,72,72	0
4	CA	A	1004	1/1	0.96	0.05	56,56,56,56	0
4	CA	A	1003	1/1	0.97	0.04	55,55,55,55	0
6	TTP	A	1010	29/29	0.98	0.05	18,30,36,38	0
4	CA	A	1001	1/1	0.99	0.01	35,35,35,35	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.