



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2026 – 04:07 PM EDT

PDB ID : 9YSI / pdb\_00009ysi  
Title : Covalent allosteric inhibitor of human DNA polymerase theta  
Authors : Mader, P.; Sicheri, F.  
Deposited on : 2025-10-18  
Resolution : 2.00 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](mailto: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

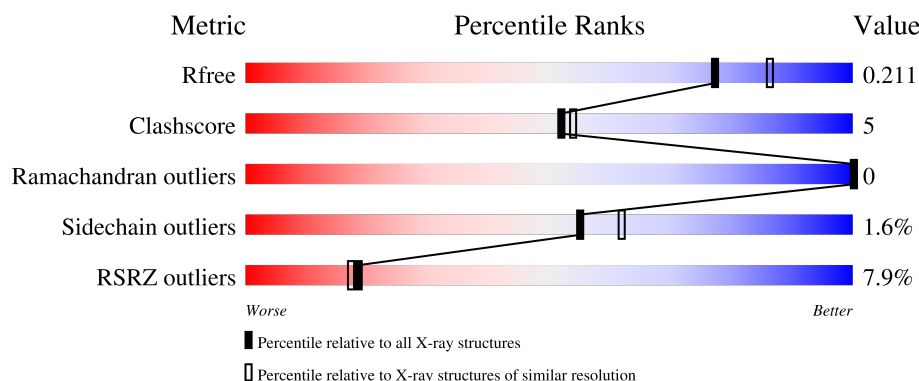
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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	668	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>
1	D	668	<div> <div>13%</div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
2	B	17	<div> <div>65%</div> <div>18%</div> <div>6%</div> <div>12%</div> </div>
2	E	17	<div> <div>71%</div> <div>6%</div> <div>24%</div> </div>
3	C	13	<div> <div>62%</div> <div>23%</div> <div>15%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	13	<div> <div>31%</div> <div>31%</div> <div>38%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	A	705	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11962 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 theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	653	Total	C	N	O	S	0	0	0
			5099	3245	870	954	30			
1	D	649	Total	C	N	O	S	0	0	0
			4839	3069	833	908	29			

There are 214 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O75417
A	?	-	ALA	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	PHE	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	ALA	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	ASP	deletion	UNP O75417
A	?	-	ASP	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	HIS	deletion	UNP O75417

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	ALA	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	VAL	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	MET	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	ASN	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	ASP	deletion	UNP O75417
A	?	-	ASN	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	VAL	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP O75417
A	?	-	VAL	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	MET	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	TYR	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	PHE	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	VAL	deletion	UNP O75417
A	?	-	ASN	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	CYS	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	ALA	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	MET	deletion	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	ALA	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	ARG	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
D	1	GLY	-	expression tag	UNP O75417
D	?	-	ALA	deletion	UNP O75417

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	THR	deletion	UNP O75417
D	?	-	ILE	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	PHE	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	ALA	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	GLU	deletion	UNP O75417
D	?	-	ILE	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	ILE	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	ASP	deletion	UNP O75417
D	?	-	ASP	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	HIS	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	GLU	deletion	UNP O75417
D	?	-	ILE	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	ALA	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	VAL	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	MET	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	ASN	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	THR	deletion	UNP O75417

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	THR	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	ILE	deletion	UNP O75417
D	?	-	ASP	deletion	UNP O75417
D	?	-	ASN	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	VAL	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	GLU	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	ALA	deletion	UNP O75417
D	?	-	VAL	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	MET	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	TYR	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	GLY	deletion	UNP O75417
D	?	-	PHE	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417

*Continued on next page...*



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP O75417
D	?	-	ASN	deletion	UNP O75417
D	?	-	PRO	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	CYS	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	ALA	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417
D	?	-	MET	deletion	UNP O75417
D	?	-	GLU	deletion	UNP O75417
D	?	-	GLU	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	ALA	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	SER	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	ARG	deletion	UNP O75417
D	?	-	LYS	deletion	UNP O75417
D	?	-	LEU	deletion	UNP O75417
D	?	-	GLN	deletion	UNP O75417

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			301	144	57	86	14			
2	E	13	Total	C	N	O	P	0	0	0
			263	126	51	74	12			

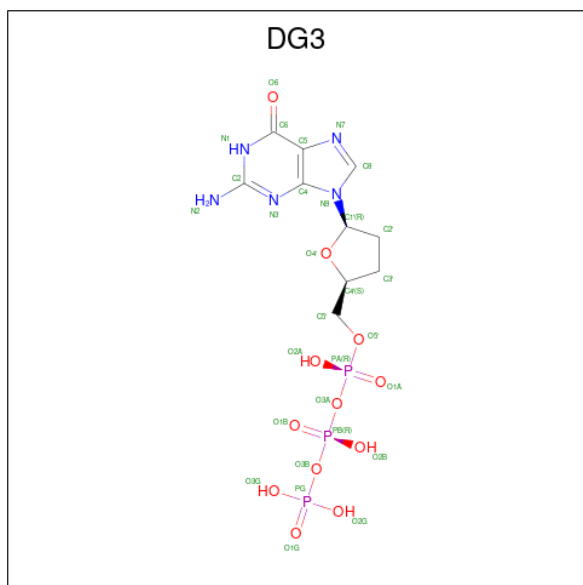
- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*G)-3').

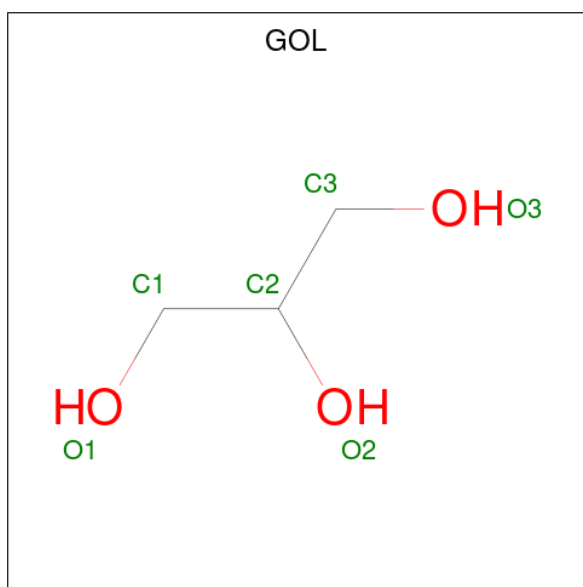
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			223	108	39	66	10			
3	F	8	Total	C	N	O	P	0	0	0
			163	79	26	50	8			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

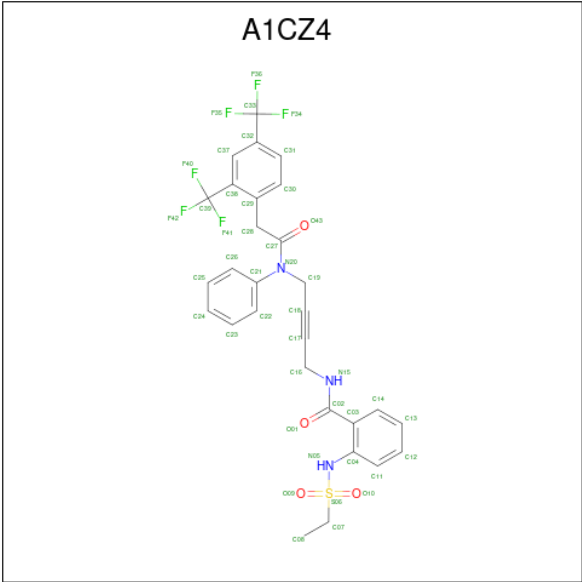
- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).





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		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is N-(4-{2-[2,4-bis(trifluoromethyl)phenyl]-N-phenylacetamido}but-2-yn-1-yl)-2-(ethanesulfonamido)benzamide (CCD ID: A1CZ4) (formula: C<sub>29</sub>H<sub>25</sub>F<sub>6</sub>N<sub>3</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	F	N	O	S	0	0
			43	29	6	3	4	1		
8	D	1	Total	C	F	N	O	S	0	0
			43	29	6	3	4	1		

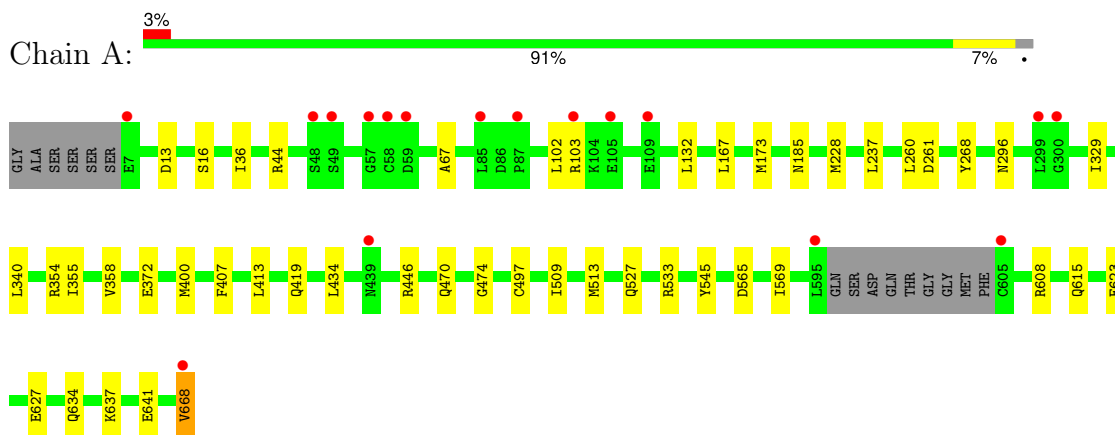
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	577	Total	O	0	0
			577	577		
9	B	51	Total	O	0	0
			51	51		
9	C	24	Total	O	0	0
			24	24		
9	D	223	Total	O	0	0
			223	223		
9	E	14	Total	O	0	0
			14	14		
9	F	3	Total	O	0	0
			3	3		

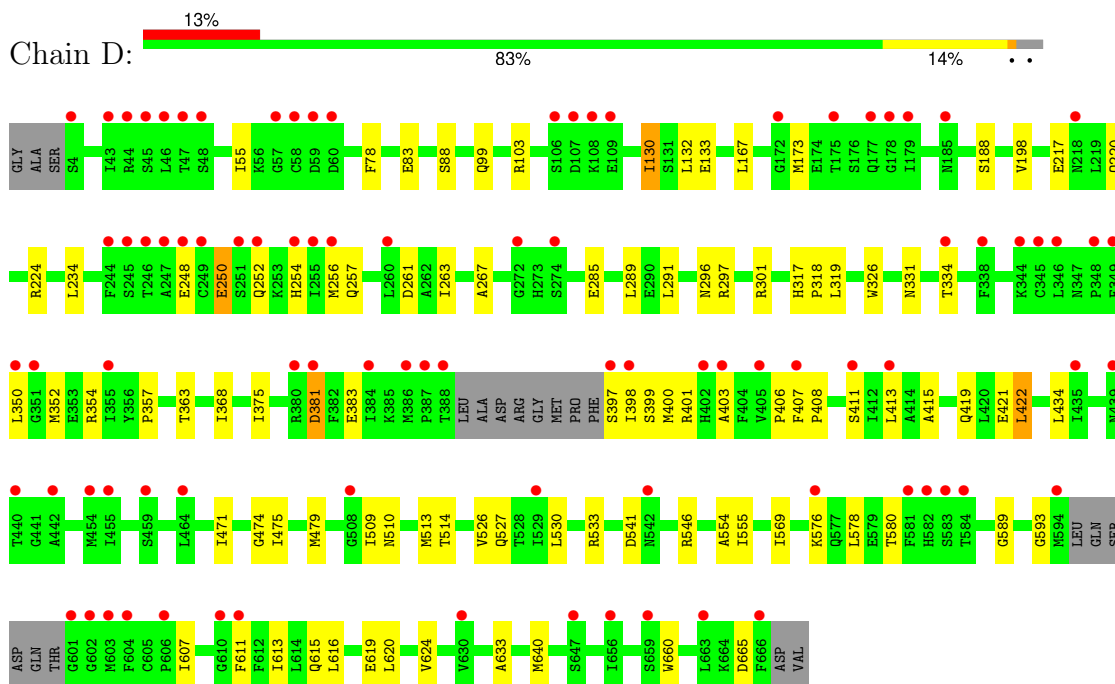
### 3 Residue-property plots [i](#)

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 theta

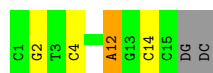


- Molecule 1: DNA polymerase theta



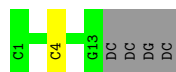
- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C)-3')

Chain B:  65% 18% 6% 12%



- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C)-3')

Chain E:  71% 6% 24%

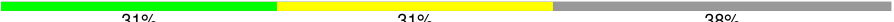


- Molecule 3: DNA (5'-D(\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*G)-3')

Chain C:  62% 23% 15%



- Molecule 3: DNA (5'-D(\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*TP\*G)-3')

Chain F:  31% 31% 38%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	248.52Å 66.62Å 151.91Å 90.00° 122.23° 90.00°	Depositor
Resolution (Å)	60.97 – 2.00 60.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (60.97-2.00) 98.1 (60.97-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, $R_{free}$	0.175 , 0.211 0.178 , 0.211	Depositor DCC
$R_{free}$ test set	7048 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CL, MG, A1CZ4, DG3

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	0.81	1/5199 (0.0%)	0.83	1/7032 (0.0%)
1	D	0.55	0/4931	0.68	0/6695
2	B	0.71	0/337	0.88	1/517 (0.2%)
2	E	0.59	0/295	0.65	0/453
3	C	0.65	0/249	0.77	0/383
3	F	0.50	0/181	0.61	0/277
All	All	0.69	1/11192 (0.0%)	0.76	2/15357 (0.0%)

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	A	0	3
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	MET	CB-CG	6.09	1.70	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	DA	C5'-C4'-C3'	-6.20	105.59	114.90
1	A	173	MET	CG-SD-CE	-5.26	89.33	100.90

There are no chirality outliers.



All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	354	ARG	Sidechain
1	A	446	ARG	Sidechain
1	D	354	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	5099	0	5049	30	0
1	D	4839	0	4555	68	0
2	B	301	0	169	5	0
2	E	263	0	147	1	0
3	C	223	0	125	3	0
3	F	163	0	91	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	30	0	12	0	0
5	D	30	0	12	1	0
6	A	3	0	0	4	0
7	A	18	0	24	4	0
7	D	12	0	16	3	0
8	A	43	0	0	0	0
8	D	43	0	0	0	0
9	A	577	0	0	8	0
9	B	51	0	0	0	0
9	C	24	0	0	2	0
9	D	223	0	0	6	0
9	E	14	0	0	1	0
9	F	3	0	0	0	0
All	All	11962	0	10200	109	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 5.

The worst 5 of 109 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)
6:A:703:CL:CL	9:A:1313:HOH:O	2.20	0.94
6:A:704:CL:CL	9:A:1295:HOH:O	2.36	0.81
1:D:350:LEU:HB3	1:D:352:MET:HE3	1.61	0.80
1:D:297:ARG:NH1	9:D:801:HOH:O	2.14	0.80
2:B:12:DA:C8	2:B:12:DA:H5''	2.19	0.77

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	649/668 (97%)	636 (98%)	13 (2%)	0	100	100
1	D	643/668 (96%)	631 (98%)	12 (2%)	0	100	100
All	All	1292/1336 (97%)	1267 (98%)	25 (2%)	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	552/586 (94%)	548 (99%)	4 (1%)	76	82
1	D	482/586 (82%)	469 (97%)	13 (3%)	39	42
All	All	1034/1172 (88%)	1017 (98%)	17 (2%)	55	62

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

Mol	Chain	Res	Type
1	D	615	GLN
1	D	665	ASP
1	D	130	ILE
1	D	188	SER
1	D	250	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	252	GLN
1	D	527	GLN
1	D	119	GLN
1	D	156	HIS
1	D	180	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](#)

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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	706	-	5,5,5	0.26	0	5,5,5	0.79	0
8	A1CZ4	A	709	1	45,45,45	2.31	16 (35%)	60,65,65	2.74	27 (45%)
7	GOL	D	704	-	5,5,5	0.43	0	5,5,5	0.64	0
8	A1CZ4	D	705	1	45,45,45	2.02	11 (24%)	60,65,65	2.33	17 (28%)
5	DG3	D	702	4	31,32,32	1.16	3 (9%)	44,50,50	1.37	4 (9%)
7	GOL	A	707	-	5,5,5	0.32	0	5,5,5	1.31	1 (20%)
7	GOL	D	703	-	5,5,5	0.36	0	5,5,5	0.80	0
5	DG3	A	702	4	31,32,32	1.17	5 (16%)	44,50,50	1.51	9 (20%)
7	GOL	A	708	-	5,5,5	0.36	0	5,5,5	0.57	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
7	GOL	A	706	-	-	4/4/4/4	-
8	A1CZ4	A	709	1	-	1/42/44/44	0/3/3/3
7	GOL	D	704	-	-	0/4/4/4	-
8	A1CZ4	D	705	1	-	4/42/44/44	0/3/3/3
5	DG3	D	702	4	-	6/22/31/31	0/3/3/3
7	GOL	A	707	-	-	4/4/4/4	-
7	GOL	D	703	-	-	4/4/4/4	-
5	DG3	A	702	4	-	4/22/31/31	0/3/3/3
7	GOL	A	708	-	-	2/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	705	A1CZ4	C27-N20	7.33	1.47	1.36
8	A	709	A1CZ4	C07-S06	6.88	1.83	1.76
8	A	709	A1CZ4	C27-N20	4.75	1.43	1.36
8	D	705	A1CZ4	C08-C07	-4.57	1.35	1.51
8	A	709	A1CZ4	C08-C07	-4.32	1.36	1.51

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	705	A1CZ4	C08-C07-S06	7.52	124.08	112.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	709	A1CZ4	C08-C07-S06	7.43	123.96	112.55
8	A	709	A1CZ4	C37-C38-C29	5.88	126.31	119.15
8	A	709	A1CZ4	C17-C16-N15	5.72	119.67	112.63
8	A	709	A1CZ4	C32-C37-C38	-5.67	114.54	123.70

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	DG3	PB-O3B-PG-O3G
5	D	702	DG3	O4'-C4'-C5'-O5'
5	D	702	DG3	C3'-C4'-C5'-O5'
7	A	708	GOL	C1-C2-C3-O3
7	D	703	GOL	O1-C1-C2-O2

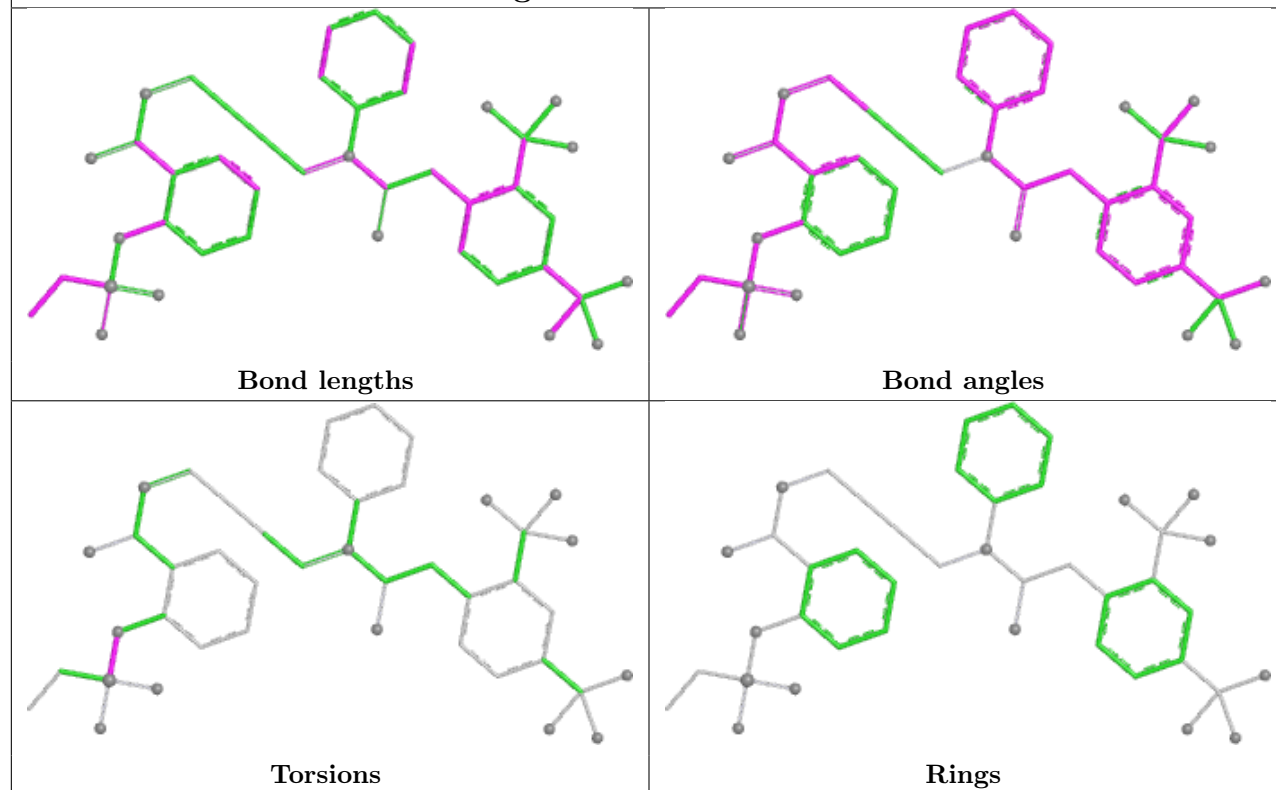
There are no ring outliers.

5 monomers are involved in 8 short contacts:

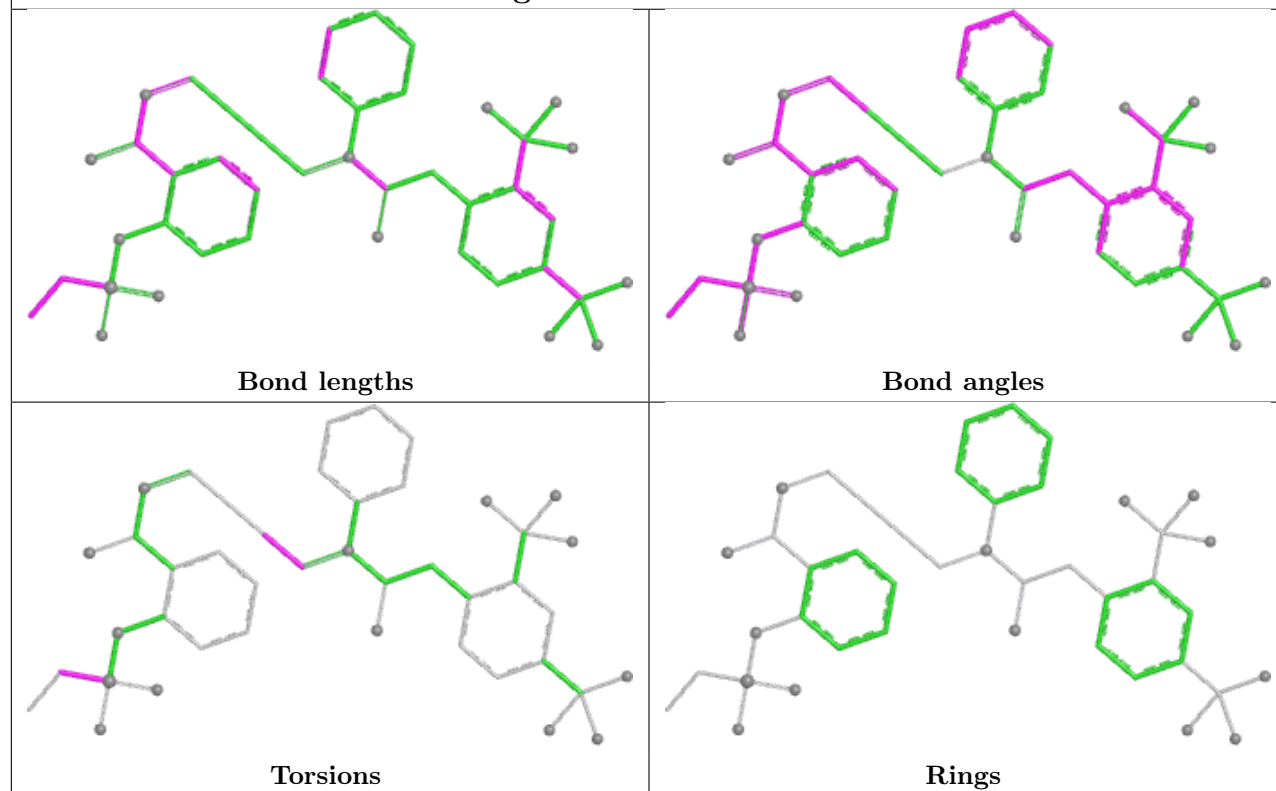
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	704	GOL	1	0
5	D	702	DG3	1	0
7	A	707	GOL	3	0
7	D	703	GOL	2	0
7	A	708	GOL	1	0

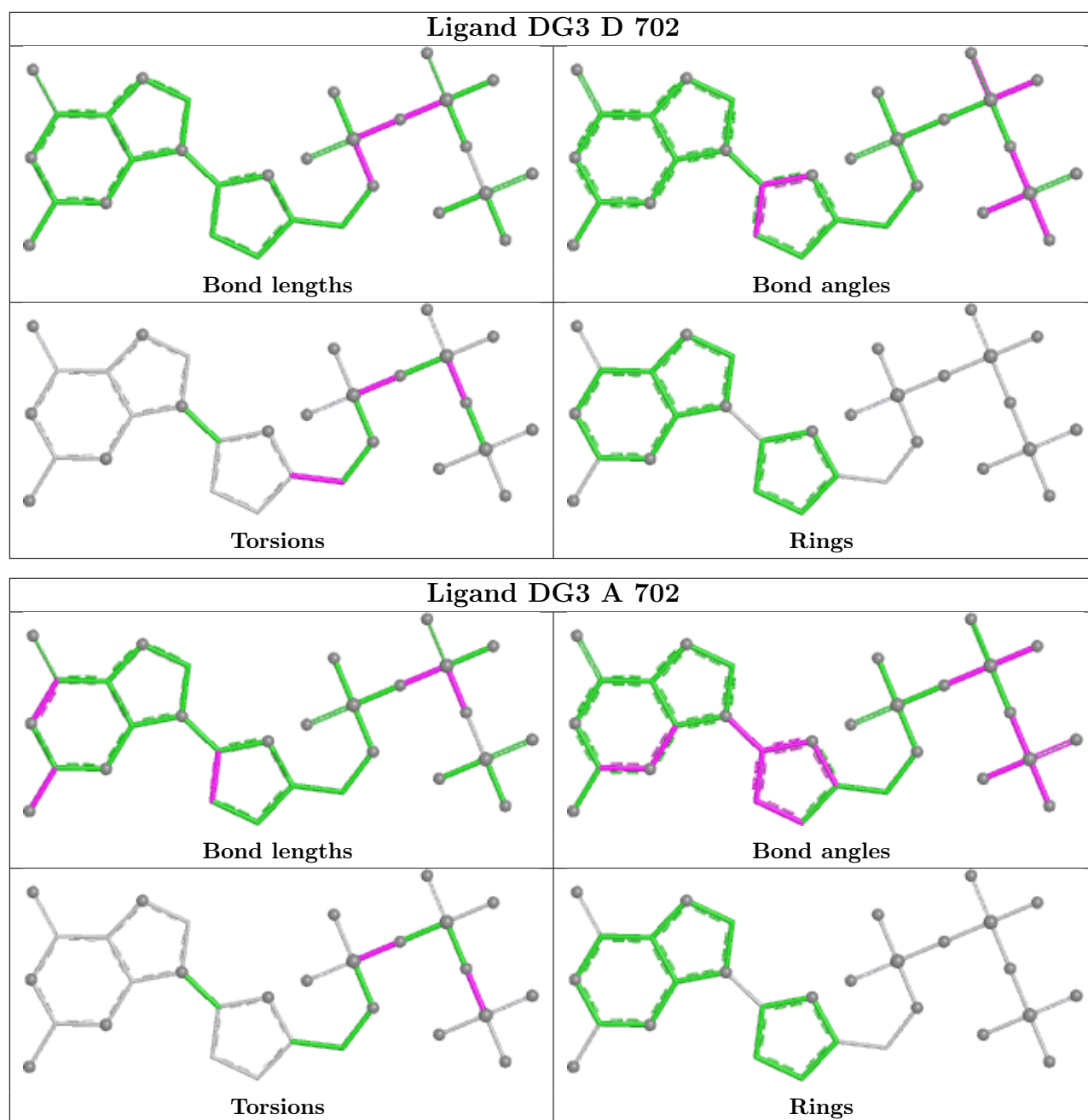
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand A1CZ4 A 709



## Ligand A1CZ4 D 705





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	653/668 (97%)	-0.13	17 (2%) 57 56	23, 38, 63, 118	0
1	D	649/668 (97%)	0.86	90 (13%) 6 5	36, 63, 97, 137	0
2	B	15/17 (88%)	-0.33	0 100 100	30, 51, 105, 133	0
2	E	13/17 (76%)	0.05	0 100 100	47, 59, 119, 140	0
3	C	11/13 (84%)	-0.02	0 100 100	30, 51, 119, 121	0
3	F	8/13 (61%)	0.29	0 100 100	60, 79, 116, 138	0
All	All	1349/1396 (96%)	0.35	107 (7%) 18 17	23, 48, 93, 140	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	PHE	5.8
1	D	604	PHE	5.8
1	D	247	ALA	5.6
1	D	601	GLY	5.5
1	D	584	THR	5.2

### 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

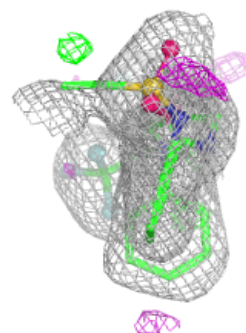
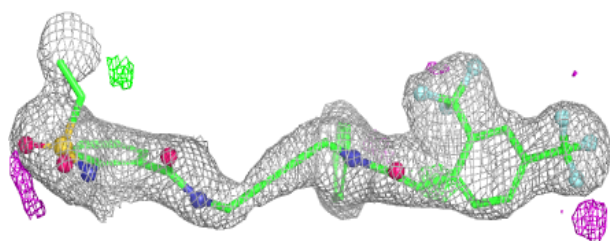
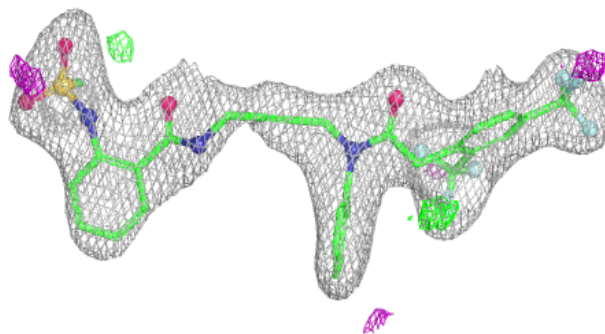
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	708	6/6	0.83	0.14	61,77,92,93	0
7	GOL	D	703	6/6	0.86	0.14	74,82,86,94	0
8	A1CZ4	D	705	43/43	0.88	0.14	55,71,92,97	0
7	GOL	A	706	6/6	0.90	0.14	61,66,73,75	0
7	GOL	D	704	6/6	0.91	0.14	52,54,55,59	0
7	GOL	A	707	6/6	0.92	0.10	35,57,63,67	0
6	CL	A	703	1/1	0.94	0.18	61,61,61,61	0
6	CL	A	704	1/1	0.94	0.20	83,83,83,83	0
6	CL	A	705	1/1	0.94	0.18	59,59,59,59	0
5	DG3	D	702	30/30	0.95	0.09	40,52,63,74	0
4	MG	D	701	1/1	0.96	0.07	63,63,63,63	0
8	A1CZ4	A	709	43/43	0.97	0.06	23,33,52,55	0
5	DG3	A	702	30/30	0.99	0.04	21,26,31,33	0
4	MG	C	101	1/1	0.99	0.06	47,47,47,47	0
4	MG	A	701	1/1	1.00	0.02	28,28,28,28	0

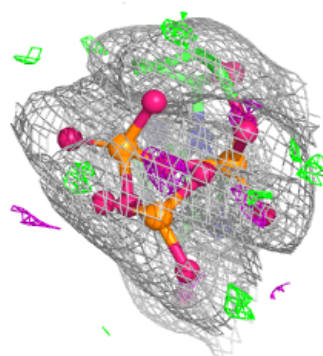
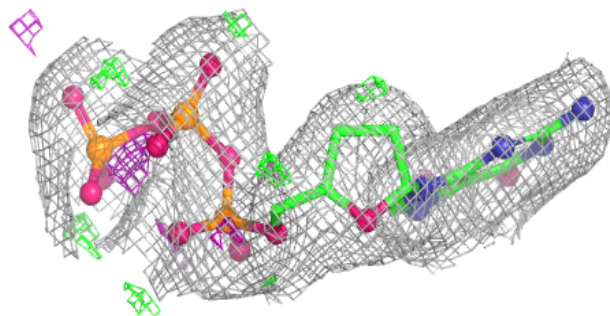
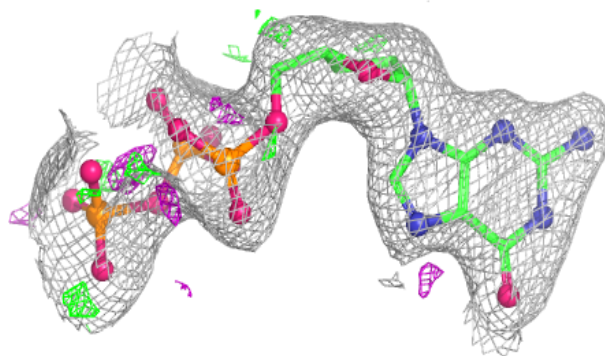
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1CZ4 D 705:**

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

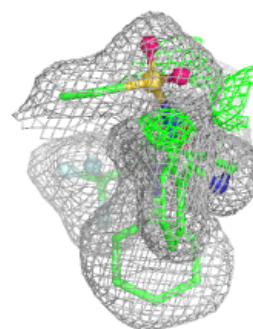
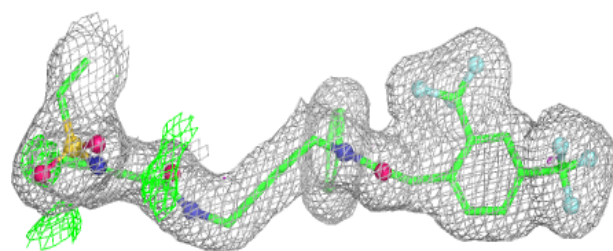
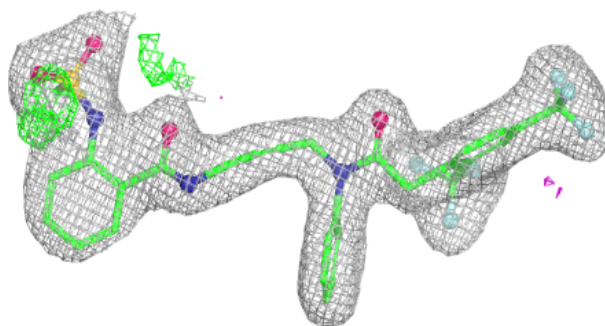
**Electron density around DG3 D 702:**

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

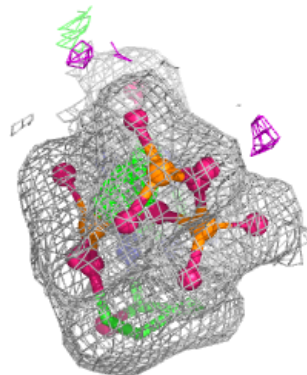
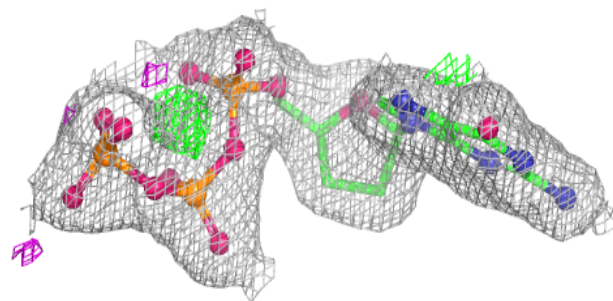
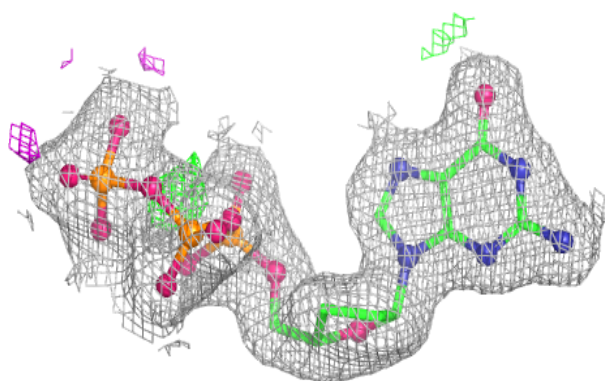


**Electron density around A1CZ4 A 709:**

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

**Electron density around DG3 A 702:**

$2mF_o-DF_c$  (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.