



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 11, 2025 – 10:07 AM EDT

PDB ID : 9D6N / pdb_00009d6n
Title : Loop-Deleted DNA Polymerase Theta in Complex with a dsDNA Overhang
and an Allosteric Inhibitor
Authors : Fried, W.; Chen, X.S.
Deposited on : 2024-08-15
Resolution : 2.43 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

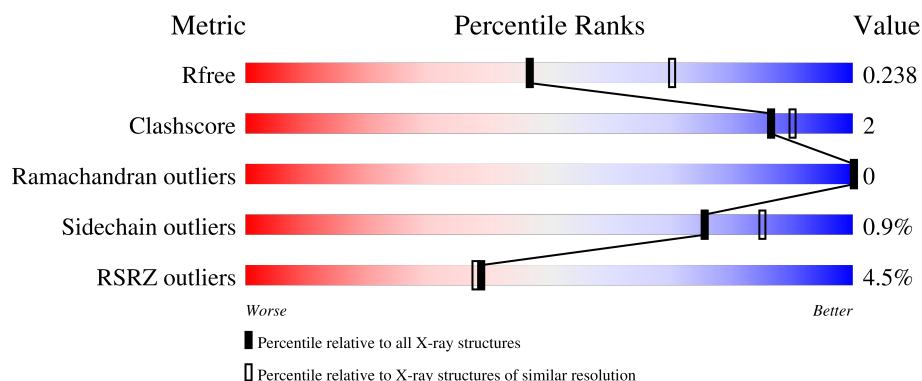
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	652	<div> <div>4%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	652	<div> <div>5%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
2	C	24	<div> <div>58%</div> <div>42%</div> </div>
2	E	24	<div> <div>83%</div> <div>17%</div> </div>
3	D	14	<div> <div>86%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	14	 71% 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12006 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	634	Total	C	N	O	S	0	0	0
			4993	3172	854	938	29			
1	B	637	Total	C	N	O	S	0	0	0
			5011	3181	860	941	29			

There are 282 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1893	GLY	-	insertion	UNP O75417
A	?	-	LEU	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	SER	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	THR	deletion	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP O75417
A	?	-	ASP	deletion	UNP O75417
A	?	-	ASP	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	?	-	PHE	deletion	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	ILE	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	GLY	deletion	UNP O75417
A	1895	GLY	CYS	conflict	UNP O75417
A	1918	GLY	GLN	conflict	UNP O75417
A	1931	GLY	LYS	conflict	UNP O75417
A	?	-	GLU	deletion	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	LYS	deletion	UNP O75417
A	?	-	HIS	deletion	UNP O75417
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	1932	SER	PRO	conflict	UNP O75417
A	1933	GLY	PRO	conflict	UNP O75417
A	1934	GLY	SER	conflict	UNP O75417
A	2146	GLY	ASN	conflict	UNP O75417
A	2172	GLY	ARG	conflict	UNP O75417
A	?	-	GLU	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	2173	SER	LEU	conflict	UNP O75417
A	2175	GLY	ARG	conflict	UNP O75417
A	?	-	PRO	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	LEU	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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	2261	GLY	ALA	conflict	UNP O75417
A	2262	GLY	ALA	conflict	UNP O75417
A	2263	SER	ASP	conflict	UNP O75417
A	2264	GLY	ARG	conflict	UNP O75417
A	?	-	GLN	deletion	UNP O75417
A	?	-	THR	deletion	UNP O75417
A	?	-	GLY	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	2522	GLY	GLN	conflict	UNP O75417
A	2524	SER	-	insertion	UNP O75417
A	2525	GLY	MET	conflict	UNP O75417
A	2526	GLY	PHE	conflict	UNP O75417
B	1893	GLY	-	insertion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	ALA	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	PHE	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	ALA	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	ASP	deletion	UNP O75417
B	?	-	ASP	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	PHE	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	1895	GLY	CYS	conflict	UNP O75417
B	1918	GLY	GLN	conflict	UNP O75417
B	1919	GLY	LYS	conflict	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	HIS	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	ALA	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	VAL	deletion	UNP O75417
B	1932	SER	PRO	conflict	UNP O75417
B	1933	GLY	PRO	conflict	UNP O75417
B	1934	GLY	SER	conflict	UNP O75417

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2171	GLY	ASN	conflict	UNP O75417
B	2172	GLY	ARG	conflict	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	MET	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	ASN	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	ILE	deletion	UNP O75417
B	?	-	ASP	deletion	UNP O75417
B	?	-	ASN	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	2173	SER	LEU	conflict	UNP O75417
B	2175	GLY	ARG	conflict	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	VAL	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	ALA	deletion	UNP O75417
B	?	-	VAL	deletion	UNP O75417

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	MET	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	TYR	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	PHE	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	VAL	deletion	UNP O75417
B	?	-	ASN	deletion	UNP O75417
B	?	-	PRO	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	CYS	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	ALA	deletion	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	MET	deletion	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	GLU	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	2261	GLY	ALA	conflict	UNP O75417
B	2262	GLY	ALA	conflict	UNP O75417
B	2263	SER	ASP	conflict	UNP O75417
B	2264	GLY	ARG	conflict	UNP O75417
B	?	-	GLN	deletion	UNP O75417
B	?	-	THR	deletion	UNP O75417
B	?	-	GLY	deletion	UNP O75417
B	?	-	LEU	deletion	UNP O75417
B	?	-	SER	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417
B	?	-	ARG	deletion	UNP O75417
B	?	-	LYS	deletion	UNP O75417

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP O75417
B	2522	GLY	GLN	conflict	UNP O75417
B	2524	SER	-	insertion	UNP O75417
B	2525	GLY	MET	conflict	UNP O75417
B	2526	GLY	PHE	conflict	UNP O75417

- Molecule 2 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			492	231	93	144	24			
2	C	24	Total	C	N	O	P	0	0	0
			492	231	93	144	24			

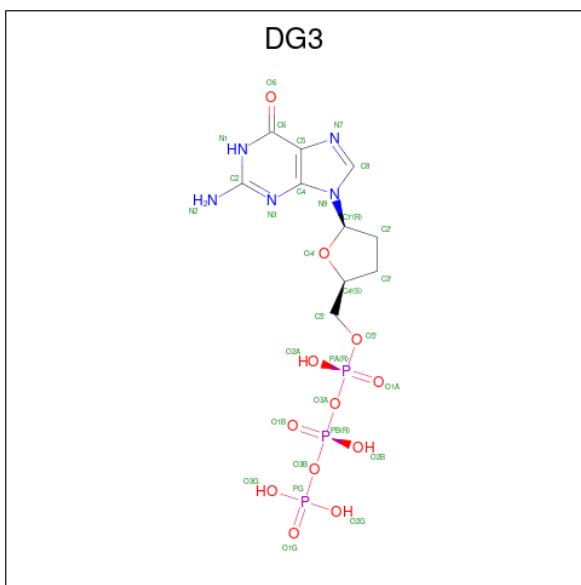
- Molecule 3 is a DNA chain called DNA Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			285	134	55	82	14			
3	D	14	Total	C	N	O	P	0	0	0
			285	134	55	82	14			

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

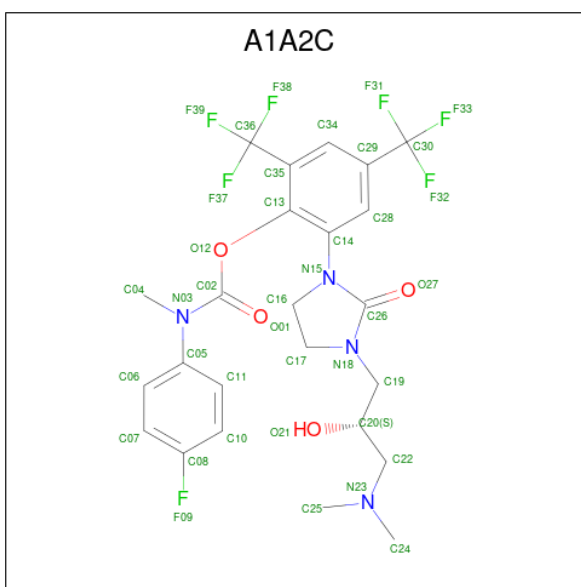
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is 2-{3-[(2R)-3-(dimethylamino)-2-hydroxypropyl]-2-oxoimidazolidin-1-yl}-4,6-bis(trifluoromethyl)phenyl (4-fluorophenyl)(methyl)carbamate (CCD ID: A1A2C) (formula: C₂₄H₂₅F₇N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			39	24	7	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	F	N	O	0	0
			39	24	7	4	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total	O	0	0
			166	166		
7	E	15	Total	O	0	0
			15	15		
7	F	11	Total	O	0	0
			11	11		
7	B	89	Total	O	0	0
			89	89		
7	C	16	Total	O	0	0
			16	16		
7	D	11	Total	O	0	0
			11	11		

Chain C:  58% 42%




• Molecule 3: DNA Primer

Chain F:  71% 29%



• Molecule 3: DNA Primer

Chain D:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.12Å 171.12Å 118.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.32 – 2.43 92.32 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.32-2.43) 100.0 (92.32-2.43)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.237 0.211 , 0.238	Depositor DCC
R_{free} test set	3794 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12006	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1A2C, MG, 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	0.11	0/5087	0.27	0/6858
1	B	0.11	0/5106	0.26	0/6884
2	C	0.18	0/551	0.34	0/848
2	E	0.17	0/551	0.36	0/848
3	D	0.17	0/319	0.33	0/489
3	F	0.16	0/319	0.37	0/489
All	All	0.12	0/11933	0.28	0/16416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4993	0	5003	21	0
1	B	5011	0	5021	15	0
2	C	492	0	268	6	1
2	E	492	0	268	3	1
3	D	285	0	154	1	0
3	F	285	0	154	2	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	30	0	12	1	0
5	B	30	0	12	1	0
6	A	39	0	0	0	0
6	B	39	0	0	0	0
7	A	166	0	0	1	0
7	B	89	0	0	0	0
7	C	16	0	0	0	0
7	D	11	0	0	0	0
7	E	15	0	0	0	0
7	F	11	0	0	0	0
All	All	12006	0	10892	45	1

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.

The worst 5 of 45 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:B:2444:LEU:HD21	1:B:2483:ILE:HD11	1.84	0.60
1:B:2369:ILE:HG22	1:B:2370:GLU:H	1.67	0.59
1:A:2002:GLU:HB3	1:A:2029:ILE:HD11	1.92	0.52
1:B:2348:LEU:HD22	1:B:2423:ILE:HD11	1.91	0.52
2:C:2:DC:H2''	2:C:3:DG:H5''	1.92	0.52

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:DC:O2	2:C:1:DG:N2[6_555]	2.19	0.01

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	624/652 (96%)	613 (98%)	11 (2%)	0	100	100
1	B	629/652 (96%)	615 (98%)	14 (2%)	0	100	100
All	All	1253/1304 (96%)	1228 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	551/561 (98%)	545 (99%)	6 (1%)	70	80
1	B	552/561 (98%)	548 (99%)	4 (1%)	81	89
All	All	1103/1122 (98%)	1093 (99%)	10 (1%)	75	85

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1955	GLU
1	B	2196	LEU
1	B	2258	ILE
1	A	2258	ILE
1	A	2308	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2055	ASN
1	A	2553	GLN
1	B	1834	GLN
1	B	2027	GLN
1	B	2040	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
6	A1A2C	B	2603	-	41,41,41	1.25	1 (2%)	59,62,62	1.31	7 (11%)
6	A1A2C	A	2603	-	41,41,41	1.25	1 (2%)	59,62,62	1.34	6 (10%)
5	DG3	A	2602	4	28,32,32	1.91	4 (14%)	33,50,50	1.11	1 (3%)
5	DG3	B	2602	4	28,32,32	2.05	4 (14%)	33,50,50	1.17	2 (6%)

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	A1A2C	B	2603	-	-	4/36/49/49	0/3/3/3
6	A1A2C	A	2603	-	-	3/36/49/49	0/3/3/3
5	DG3	A	2602	4	-	0/18/31/31	0/3/3/3
5	DG3	B	2602	4	-	6/18/31/31	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2602	DG3	PB-O3A	8.55	1.68	1.59
5	A	2602	DG3	PB-O3A	7.87	1.68	1.59
6	B	2603	A1A2C	C02-N03	5.93	1.48	1.36
6	A	2603	A1A2C	C02-N03	5.89	1.48	1.36
5	B	2602	DG3	PA-O3A	3.59	1.63	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2603	A1A2C	C16-N15-C26	-3.96	108.66	111.77
6	A	2603	A1A2C	C17-C16-N15	3.66	107.88	102.86
6	B	2603	A1A2C	C16-N15-C26	-3.13	109.32	111.77
5	B	2602	DG3	O4'-C4'-C5'	3.06	114.86	109.34
6	B	2603	A1A2C	C17-C16-N15	2.97	106.94	102.86

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2602	DG3	O4'-C4'-C5'-O5'
5	B	2602	DG3	C3'-C4'-C5'-O5'
6	A	2603	A1A2C	N18-C19-C20-C22
6	A	2603	A1A2C	C20-C22-N23-C24
6	A	2603	A1A2C	N18-C19-C20-O21

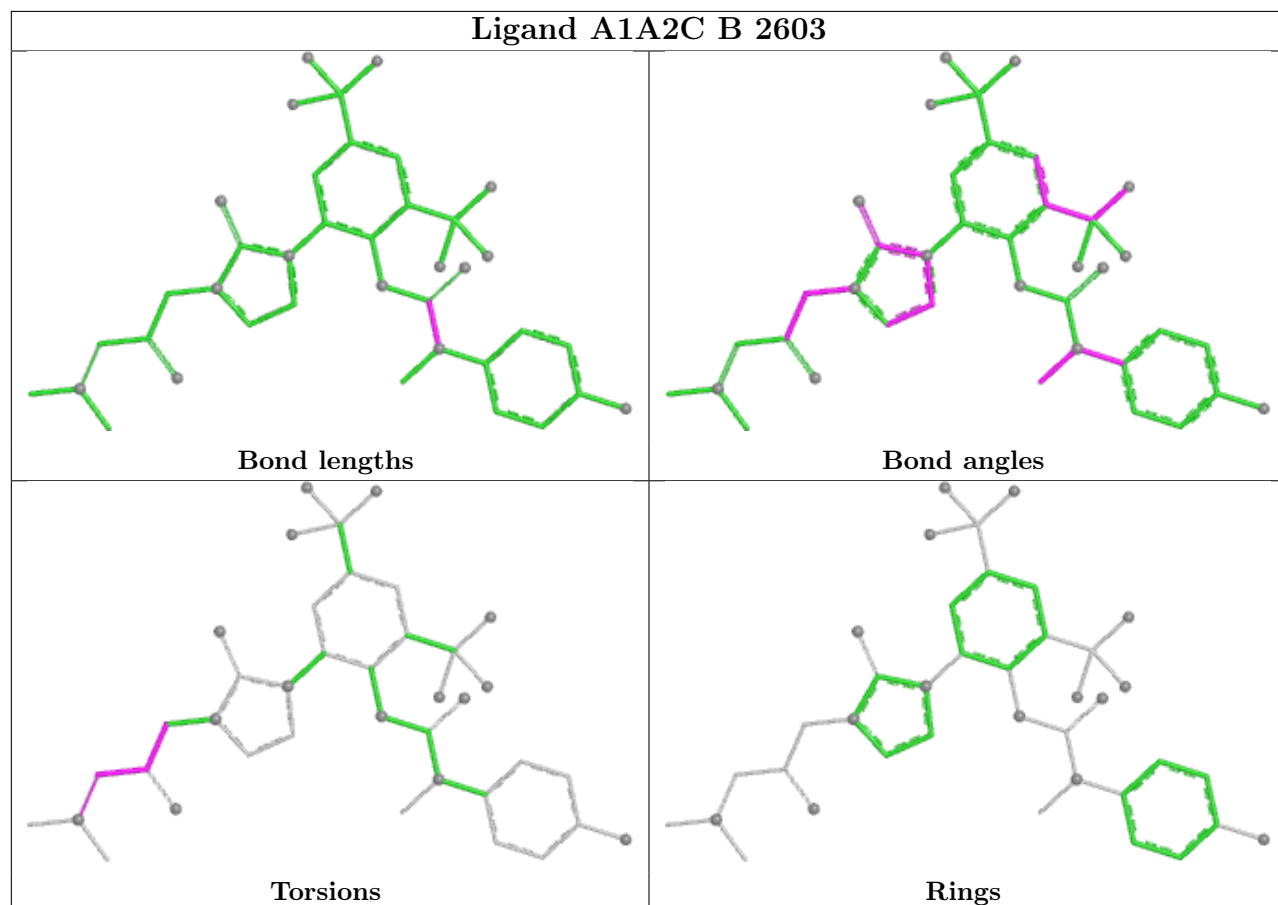
There are no ring outliers.

2 monomers are involved in 2 short contacts:

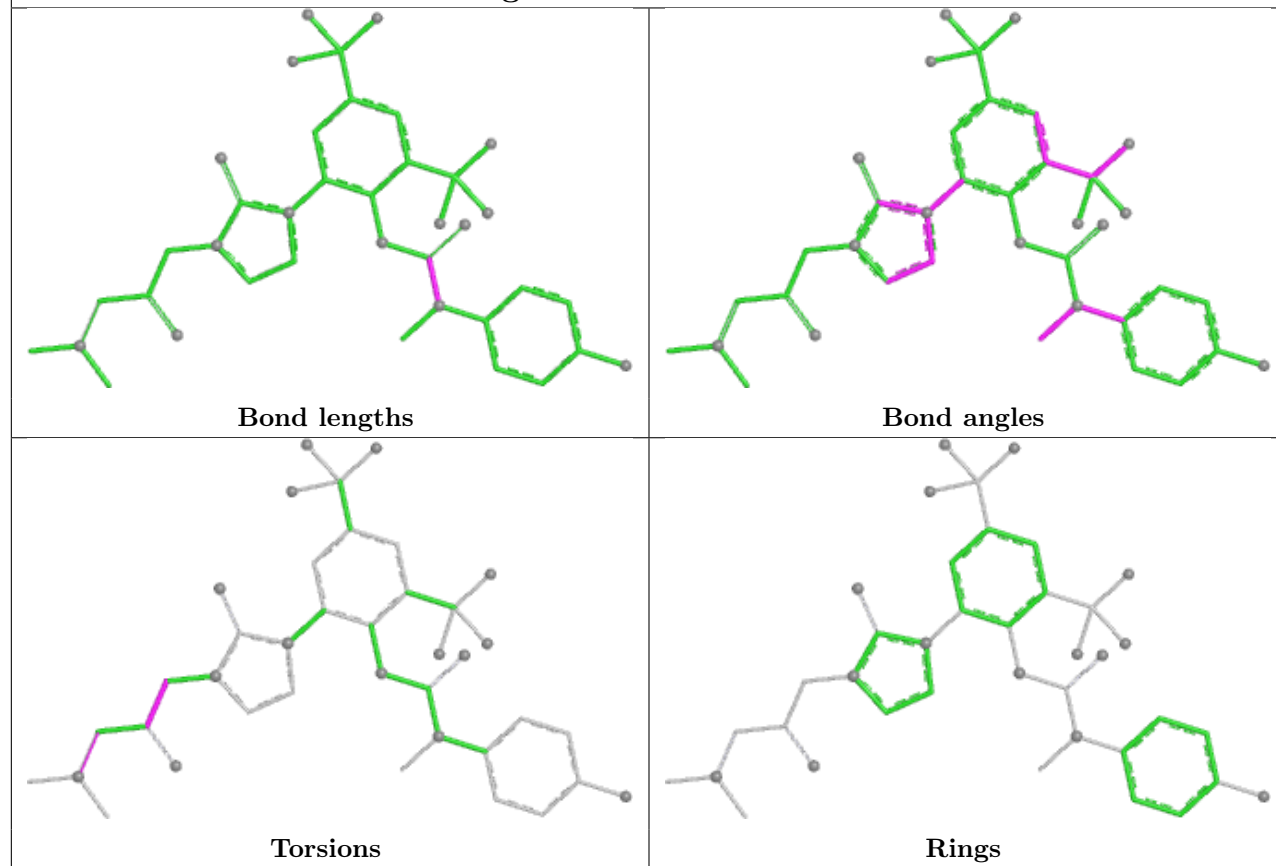
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2602	DG3	1	0
5	B	2602	DG3	1	0

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

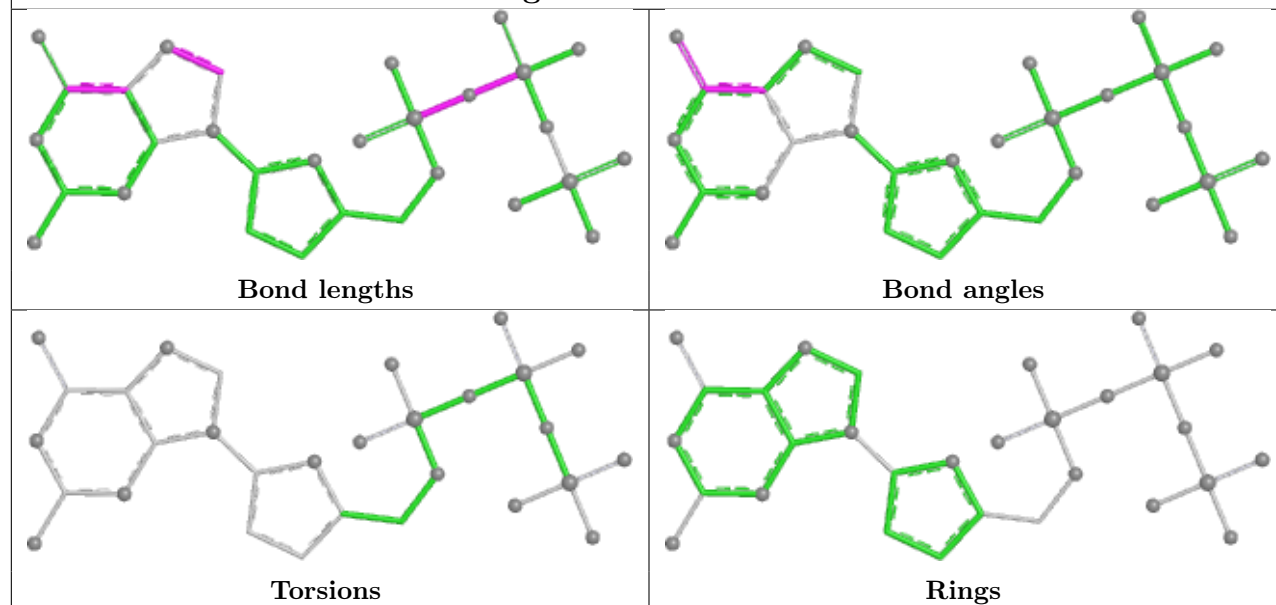
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

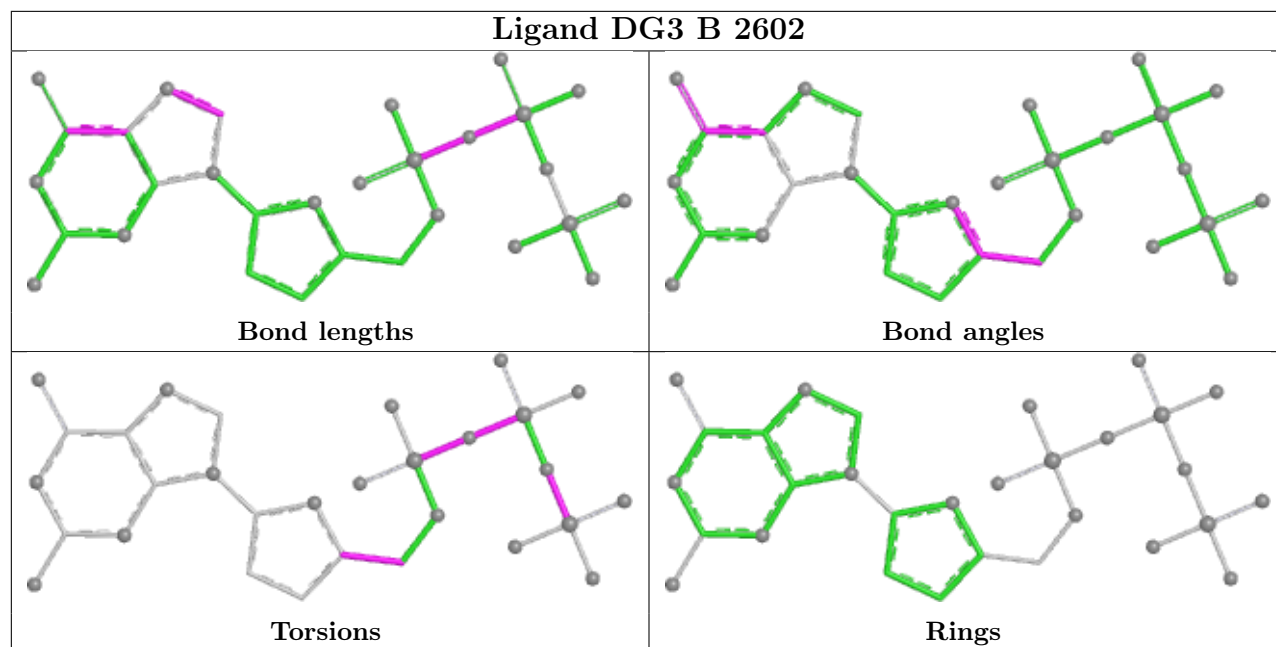


Ligand A1A2C A 2603



Ligand DG3 A 2602





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	A	634/652 (97%)	0.19	29 (4%) 38 37	40, 60, 113, 151	0
1	B	637/652 (97%)	0.43	32 (5%) 35 34	42, 69, 120, 168	0
2	C	24/24 (100%)	0.16	0 100 100	48, 99, 152, 158	0
2	E	24/24 (100%)	0.22	0 100 100	43, 112, 158, 198	0
3	D	14/14 (100%)	0.07	0 100 100	50, 83, 173, 190	0
3	F	14/14 (100%)	0.10	0 100 100	42, 83, 168, 187	0
All	All	1347/1380 (97%)	0.30	61 (4%) 39 38	40, 65, 124, 198	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2026	SER	5.1
1	A	1859	ILE	4.7
1	A	2175	GLY	4.0
1	B	2525	GLY	3.9
1	B	2029	ILE	3.8

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](#)

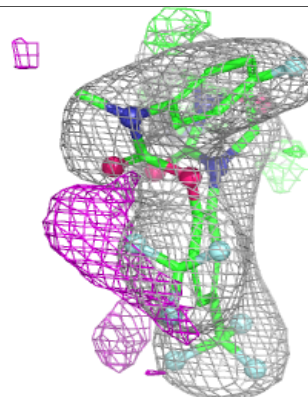
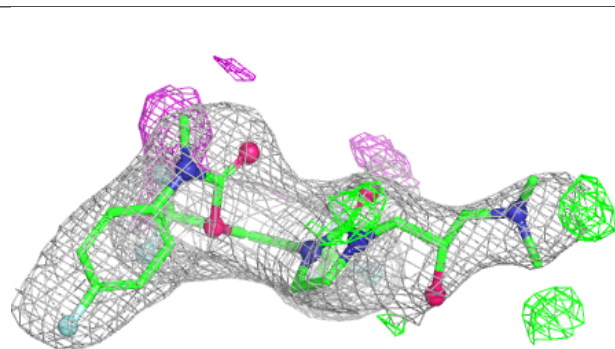
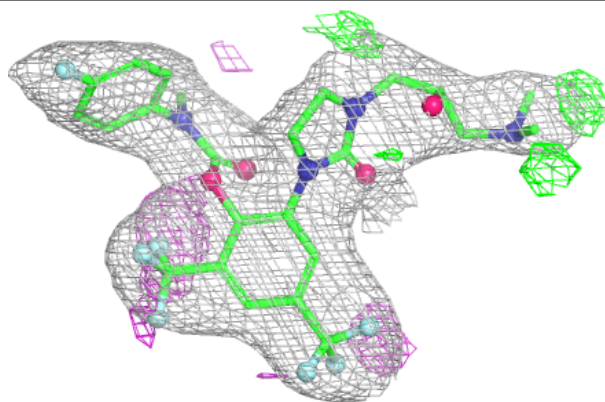
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	2601	1/1	0.85	0.23	62,62,62,62	0
6	A1A2C	B	2603	39/39	0.88	0.14	59,71,90,94	0
4	MG	A	2601	1/1	0.91	0.24	54,54,54,54	0
6	A1A2C	A	2603	39/39	0.92	0.12	53,60,87,97	0
5	DG3	B	2602	30/30	0.95	0.08	46,54,67,73	0
5	DG3	A	2602	30/30	0.96	0.07	41,43,60,84	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.

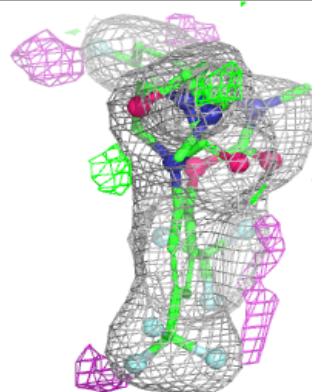
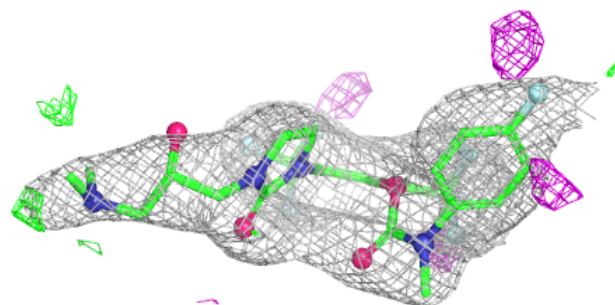
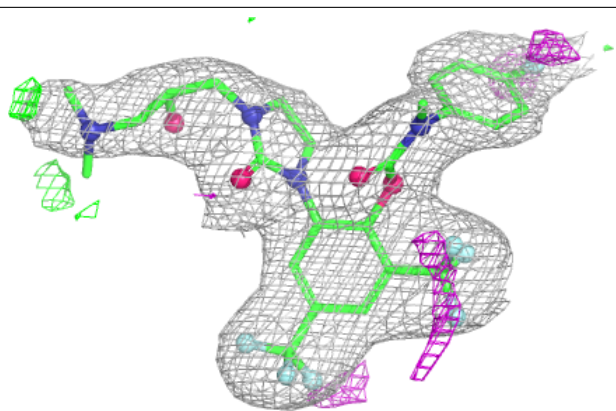
Electron density around A1A2C B 2603:

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

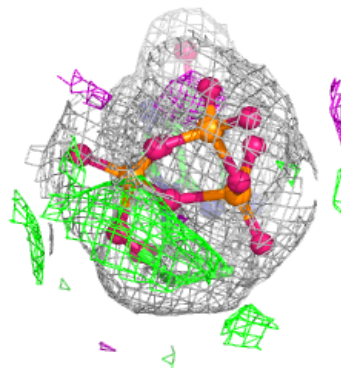
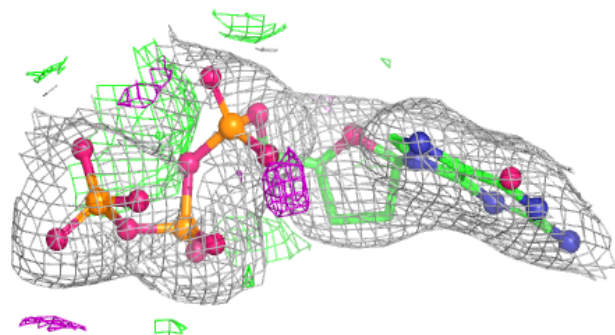
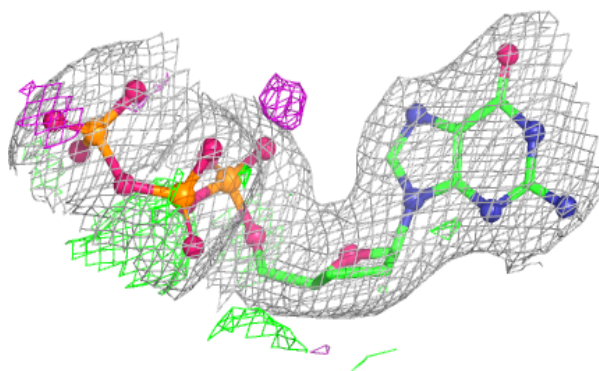


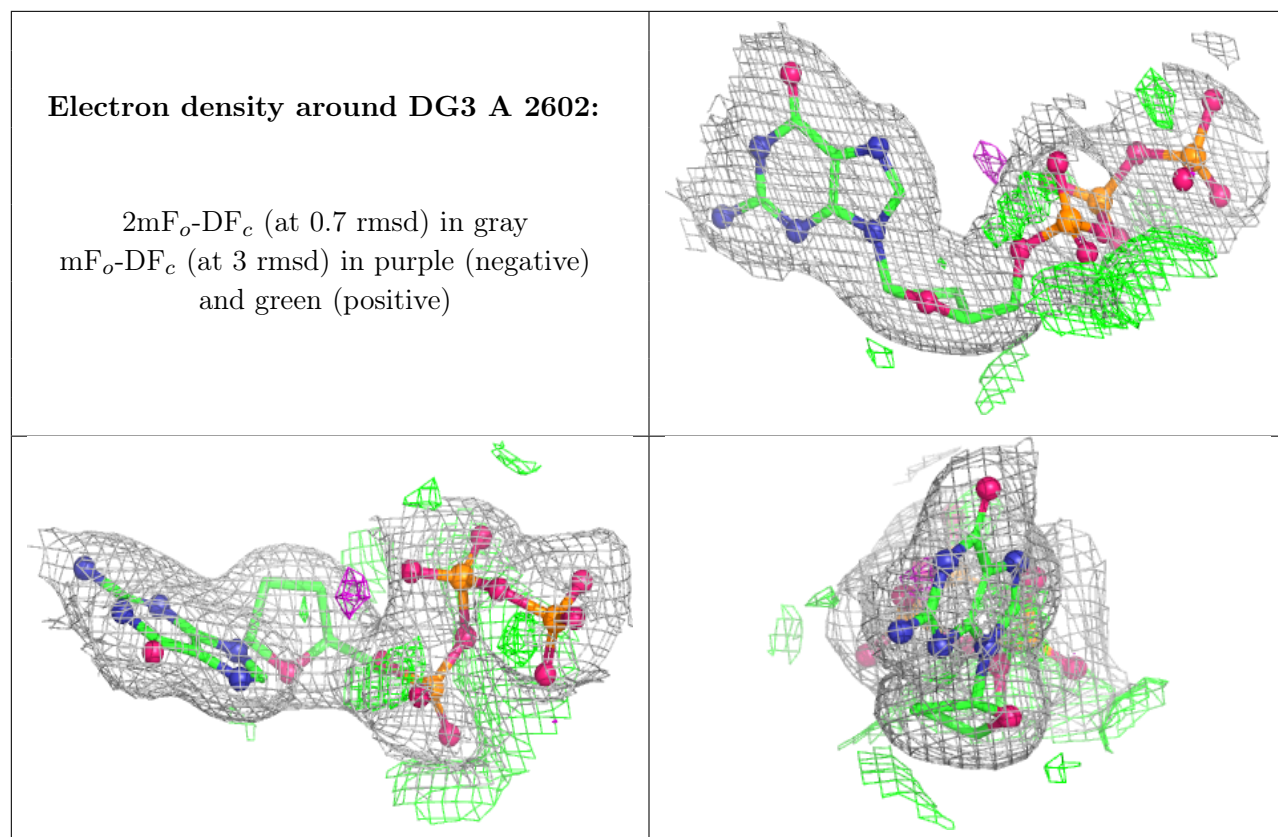
Electron density around A1A2C A 2603:

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

**Electron density around DG3 B 2602:**

$2mF_o-DF_c$ (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.