



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:53 AM UTC

PDB ID : 8E23 / pdb_00008e23
Title : Human DNA polymerase theta in complex with allosteric inhibitor
Authors : Mader, P.; Pau, V.P.T.; Sicheri, F.
Deposited on : 2022-08-13
Resolution : 2.59 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

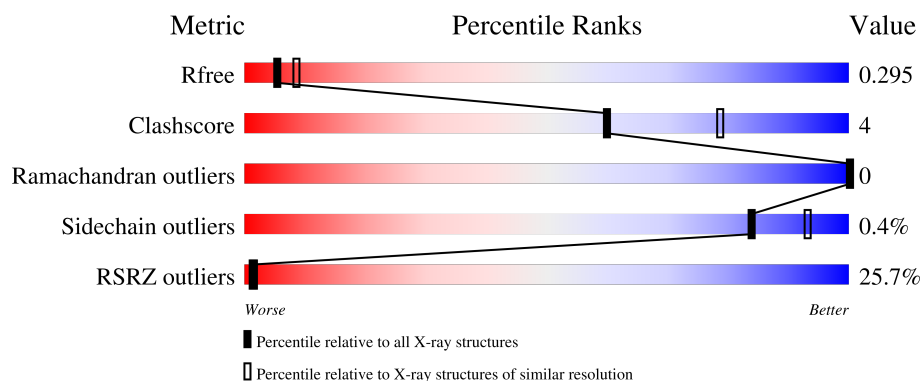
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	668	7% 88% 8% 5%
1	D	668	42% 78% 12% 10%
2	B	17	82% 6% 12%
2	E	17	53% 18% 29%
3	C	13	8% 62% 23% 15%

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Mol	Chain	Length	Quality of chain
3	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left representing 46%, a yellow segment in the middle representing 15%, and a grey segment on the right representing 38%. The percentages are labeled below their respective segments.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10562 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	637	Total	C	N	O	S	0	0	0
			4980	3171	855	927	27			
1	D	603	Total	C	N	O	S	0	0	0
			4478	2819	775	862	22			

There are 214 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1817	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

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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

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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	1817	GLY	-	expression tag	UNP O75417
D	?	-	ALA	deletion	UNP O75417

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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

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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

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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*CP*GP*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	12	Total	C	N	O	P	0	0	0
			241	116	46	68	11			

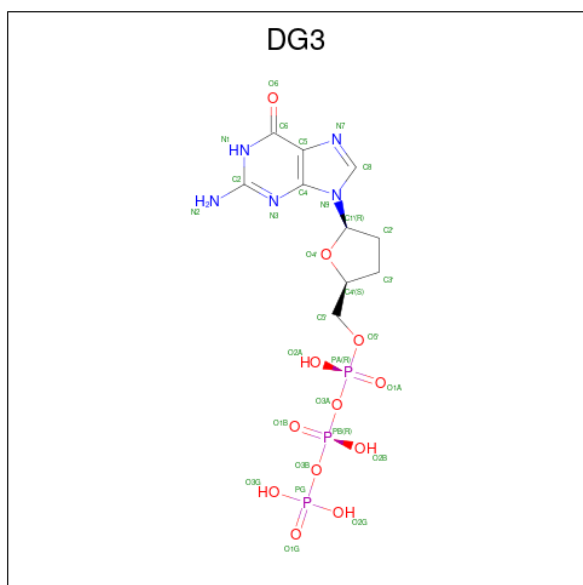
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*C*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*G)-3').

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).

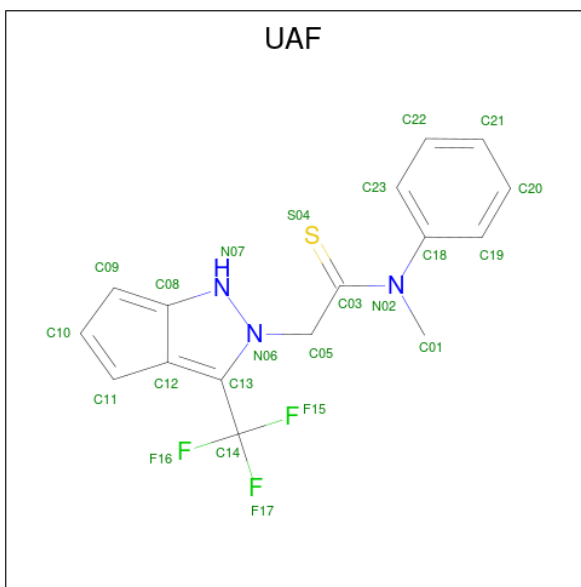
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- 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
5	A	1	Total C N O P 30 10 5 12 3	0	0
5	D	1	Total C N O P 30 10 5 12 3	0	0

- Molecule 6 is N-methyl-N-phenyl[(3aM)-3-(trifluoromethyl)cyclopenta[c]pyrazol-2(1H)-yl]ethanethioamide (CCD ID: UAF) (formula: $C_{16}H_{14}F_3N_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	S	0	0
			23	16	3	3	1		

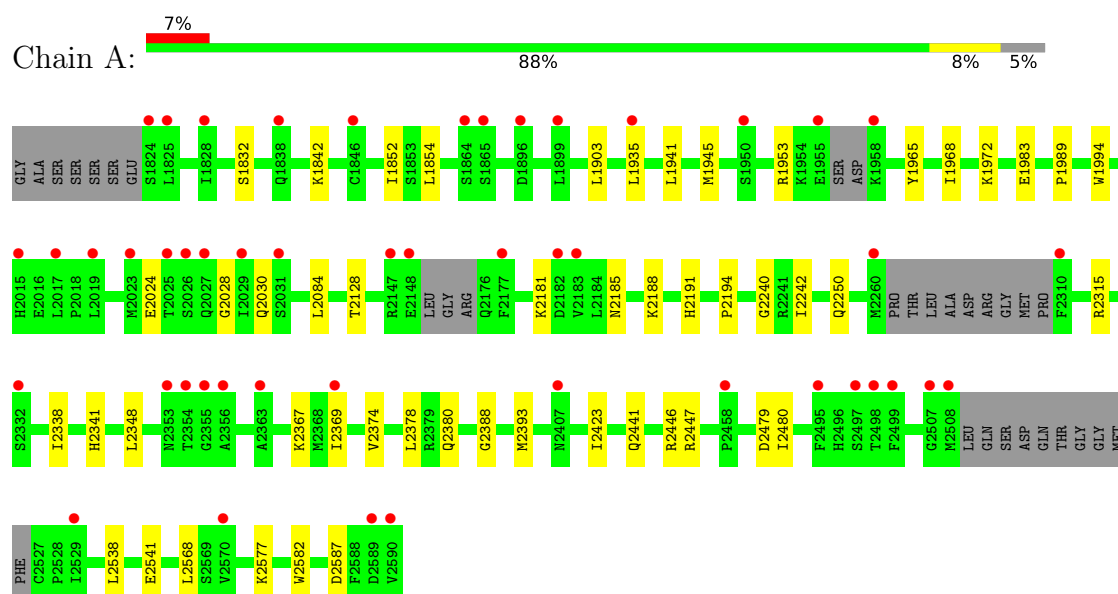
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	67	Total	O	0	0
			67	67		
7	C	4	Total	O	0	0
			4	4		
7	D	19	Total	O	0	0
			19	19		
7	E	1	Total	O	0	0
			1	1		

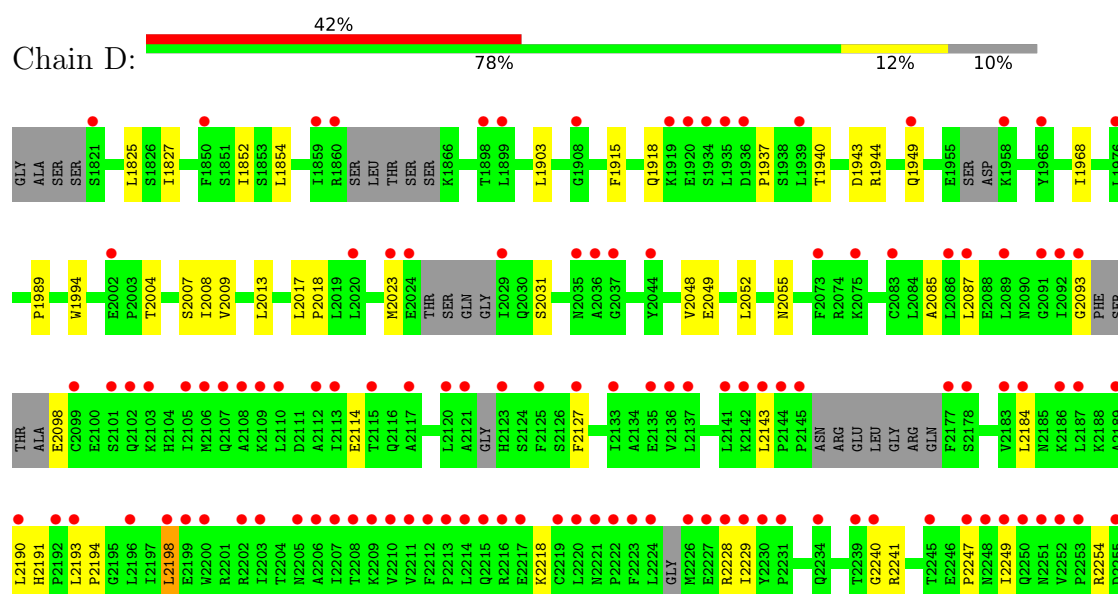
3 Residue-property plots [i](#)

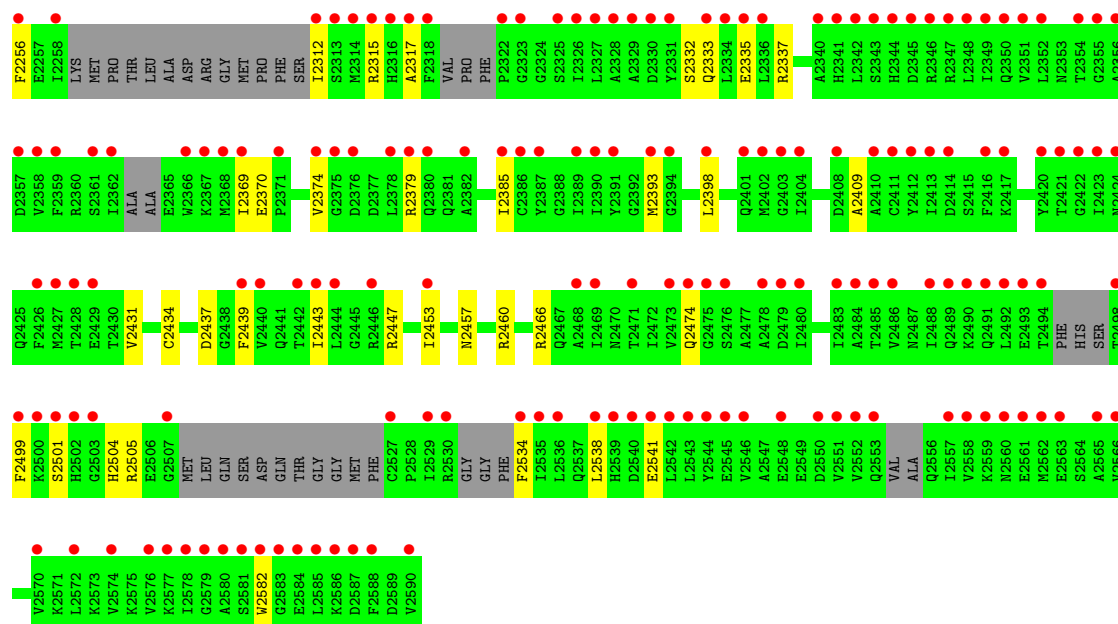
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





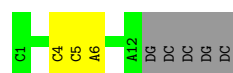
- Molecule 2: DNA (5'-D(*CP*GP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain B: 82% 6% 12%



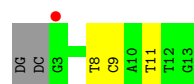
- Molecule 2: DNA (5'-D(*CP*GP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')

Chain E: 53% 18% 29%



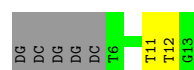
- Molecule 3: DNA (5'-D(*GP*C*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*G)-3')

Chain C: 8% 62% 23% 15%



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

Chain F: 46% 15% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.85Å 69.32Å 147.43Å 90.00° 122.55° 90.00°	Depositor
Resolution (Å)	73.53 – 2.59 73.53 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (73.53-2.59) 98.8 (73.53-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.247 , 0.295 0.248 , 0.295	Depositor DCC
R_{free} test set	1963 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10562	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: DG3, UAF, MG

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	0.06	0/5074	0.20	0/6856
1	D	0.07	0/4549	0.21	0/6163
2	B	0.13	0/337	0.26	0/517
2	E	0.15	0/270	0.30	0/414
3	C	0.14	0/249	0.36	0/383
3	F	0.17	0/181	0.39	0/277
All	All	0.08	0/10660	0.22	0/14610

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	4980	0	4940	31	0
1	D	4478	0	4136	51	0
2	B	301	0	169	1	0
2	E	241	0	136	5	0
3	C	223	0	125	2	0
3	F	163	0	91	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	30	0	12	0	0
5	D	30	0	12	1	0
6	A	23	0	0	0	0
7	A	67	0	0	2	0
7	C	4	0	0	0	0
7	D	19	0	0	0	0
7	E	1	0	0	0	0
All	All	10562	0	9621	86	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 4.

All (86) 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:D:2393:MET:HA	2:E:4:DC:H5'	1.73	0.69
1:A:1852:ILE:HB	1:A:1903:LEU:HD11	1.73	0.69
1:D:2241:ARG:HH21	1:D:2474:GLN:HB2	1.58	0.68
1:A:1854:LEU:HD23	1:A:1903:LEU:HD13	1.74	0.67
1:D:2241:ARG:NH2	1:D:2335:GLU:OE2	2.28	0.66
1:D:1852:ILE:HB	1:D:1903:LEU:HD11	1.76	0.66
1:A:1842:LYS:HE3	1:D:1937:PRO:HG2	1.80	0.64
1:D:2466:ARG:HH11	2:E:4:DC:H5''	1.63	0.64
1:D:2218:LYS:HA	1:D:2229:ILE:HG12	1.83	0.61
1:D:2004:THR:H	1:D:2007:SER:HB3	1.67	0.59
1:A:1953:ARG:HE	1:A:1983:GLU:HG3	1.69	0.58
1:D:1854:LEU:HD23	1:D:1903:LEU:HD13	1.86	0.58
1:D:2143:LEU:HD22	1:D:2190:LEU:HD13	1.86	0.57
1:D:1940:THR:OG1	1:D:1943:ASP:OD1	2.23	0.56
1:D:2256:PHE:O	1:D:2312:ILE:N	2.39	0.56
1:D:2332:SER:HB2	1:D:2337:ARG:HH21	1.71	0.55
1:D:2538:LEU:HB2	1:D:2541:GLU:HB3	1.88	0.55
1:D:2184:LEU:HB3	1:D:2198:LEU:HD11	1.89	0.55
1:D:1918:GLN:O	1:D:1944:ARG:NH2	2.36	0.54
1:D:2315:ARG:HB3	1:D:2582:TRP:HB3	1.87	0.54
1:D:2023:MET:HE1	1:D:2048:VAL:HG11	1.90	0.54
1:D:2098:GLU:HB2	1:D:2317:ALA:HB2	1.89	0.54
1:D:2241:ARG:NE	1:D:2474:GLN:OE1	2.43	0.51
1:D:2431:VAL:HG13	1:D:2453:ILE:HD11	1.91	0.51
2:E:5:DC:H2'	2:E:6:DA:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1903:LEU:O	1:D:1915:PHE:N	2.38	0.51
1:A:2185:ASN:HA	1:A:2188:LYS:HD3	1.93	0.51
1:D:2254:ARG:HH21	1:D:2379:ARG:HH21	1.58	0.50
1:D:2332:SER:O	1:D:2337:ARG:NE	2.41	0.50
3:F:11:DT:H2'	3:F:12:DT:C6	2.47	0.50
1:A:2348:LEU:HD22	1:A:2423:ILE:HD11	1.93	0.50
1:D:2466:ARG:NH1	2:E:4:DC:H5''	2.28	0.49
1:D:2093:GLY:HA2	1:D:2228:ARG:HG2	1.94	0.49
1:A:2028:GLY:O	1:A:2030:GLN:N	2.43	0.48
1:A:2084:LEU:HD11	1:A:2242:ILE:HD13	1.96	0.47
1:A:2181:LYS:NZ	3:C:11:DT:OP2	2.45	0.47
1:A:2538:LEU:HB3	1:A:2541:GLU:HB3	1.95	0.47
1:D:2247:PRO:HG2	1:D:2249:ILE:HD11	1.97	0.47
1:D:2499:PHE:CE2	1:D:2505:ARG:HG2	2.50	0.47
1:A:2341:HIS:CD2	1:A:2568:LEU:HD22	2.49	0.47
1:D:2333:GLN:NE2	5:D:2601:DG3:O1G	2.47	0.47
2:E:5:DC:H2'	2:E:6:DA:C8	2.50	0.47
1:D:2439:PHE:HB2	1:D:2447:ARG:HB3	1.96	0.47
1:D:2013:LEU:HD11	1:D:2055:ASN:HB2	1.96	0.46
1:A:2441:GLN:HG2	1:A:2447:ARG:HG2	1.97	0.46
1:D:2191:HIS:O	1:D:2194:PRO:HD2	2.14	0.46
1:D:2398:LEU:HD23	1:D:2409:ALA:HB1	1.96	0.46
1:A:1941:LEU:O	1:A:1945:MET:HG2	2.16	0.45
1:A:2338:ILE:HD11	1:A:2480:ILE:HD12	1.98	0.45
1:D:1989:PRO:HB2	1:D:2008:ILE:HD13	1.98	0.45
1:D:2114:GLU:HG2	1:D:2127:PHE:CE1	2.51	0.45
1:A:1965:TYR:HD1	1:A:1989:PRO:HG2	1.82	0.45
1:A:2388:GLY:HA3	1:A:2393:MET:HE3	1.99	0.44
1:A:2446:ARG:NH1	1:A:2479:ASP:OD1	2.50	0.44
1:D:2315:ARG:HD3	1:D:2582:TRP:CD2	2.52	0.44
1:A:2369:ILE:HD11	1:A:2374:VAL:HG22	1.98	0.44
3:F:11:DT:H2'	3:F:12:DT:H6	1.82	0.44
1:D:1968:ILE:HG12	1:D:2085:ALA:HB2	2.00	0.44
1:A:2446:ARG:NH2	7:A:2707:HOH:O	2.51	0.43
1:D:2385:ILE:HG23	1:D:2398:LEU:HD11	2.00	0.43
1:D:2434:CYS:HA	1:D:2437:ASP:O	2.18	0.43
1:D:1994:TRP:HZ2	1:D:2240:GLY:HA2	1.82	0.43
1:A:1994:TRP:HZ2	1:A:2240:GLY:HA2	1.84	0.43
1:A:2128:THR:HB	2:B:12:DA:H5'	2.01	0.43
1:D:2009:VAL:HG21	1:D:2052:LEU:HD13	2.00	0.43
1:A:2191:HIS:O	1:A:2194:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2315:ARG:HB3	1:A:2582:TRP:HB3	2.00	0.42
1:A:2367:LYS:HG3	1:A:2378:LEU:HD21	2.01	0.42
1:A:1832:SER:HB2	1:A:1935:LEU:HD12	2.02	0.42
1:A:2577:LYS:HG2	1:A:2587:ASP:HA	2.02	0.42
1:D:2501:SER:O	1:D:2505:ARG:HG3	2.18	0.42
1:A:2024:GLU:H	1:A:2024:GLU:CD	2.28	0.42
1:D:2017:LEU:N	1:D:2018:PRO:HD2	2.34	0.42
1:D:2031:SER:HG	1:D:2049:GLU:CD	2.28	0.42
1:A:1994:TRP:CZ2	1:A:2240:GLY:HA2	2.55	0.41
1:D:1825:LEU:HD23	1:D:1827:ILE:HD11	2.02	0.41
1:D:2457:ASN:HB3	1:D:2460:ARG:HB2	2.02	0.41
1:D:2193:LEU:HB3	1:D:2194:PRO:HD3	2.03	0.41
1:D:2369:ILE:HG12	1:D:2370:GLU:H	1.85	0.41
1:A:1968:ILE:O	1:A:1972:LYS:HG3	2.20	0.41
3:C:8:DT:H2"	3:C:9:DC:C6	2.56	0.41
1:D:2194:PRO:O	1:D:2198:LEU:HD12	2.21	0.41
1:D:2501:SER:HB3	1:D:2504:HIS:HB2	2.02	0.41
1:A:2250:GLN:HG2	1:A:2538:LEU:HD12	2.04	0.40
1:A:2380:GLN:NE2	7:A:2709:HOH:O	2.54	0.40
1:D:2087:LEU:HD12	1:D:2534:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	627/668 (94%)	612 (98%)	15 (2%)	0	100	100
1	D	575/668 (86%)	554 (96%)	21 (4%)	0	100	100
All	All	1202/1336 (90%)	1166 (97%)	36 (3%)	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	539/586 (92%)	539 (100%)	0	100	100
1	D	446/586 (76%)	442 (99%)	4 (1%)	70	87
All	All	985/1172 (84%)	981 (100%)	4 (0%)	84	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1949	GLN
1	D	2198	LEU
1	D	2374	VAL
1	D	2443	ILE

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	2474	GLN
1	D	1949	GLN
1	D	2185	ASN
1	D	2381	GLN
1	D	2467	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
5	DG3	A	2601	4	31,32,32	1.23	3 (9%)	44,50,50	1.87	7 (15%)
6	UAF	A	2602	-	22,25,25	3.55	10 (45%)	23,37,37	1.47	6 (26%)
5	DG3	D	2601	4	31,32,32	1.21	3 (9%)	44,50,50	1.89	7 (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
5	DG3	A	2601	4	-	5/22/31/31	0/3/3/3
6	UAF	A	2602	-	-	1/17/18/18	0/3/3/3
5	DG3	D	2601	4	-	6/22/31/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2602	UAF	C10-C11	10.32	1.56	1.37
6	A	2602	UAF	C05-N06	6.18	1.56	1.46
6	A	2602	UAF	C05-C03	6.04	1.59	1.52
6	A	2602	UAF	C09-C08	4.84	1.54	1.41
6	A	2602	UAF	C03-S04	-3.83	1.58	1.66
6	A	2602	UAF	C18-N02	3.70	1.50	1.43
5	D	2601	DG3	C5-C4	3.17	1.47	1.38
5	A	2601	DG3	C5-C4	3.16	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2602	UAF	C10-C09	2.78	1.56	1.42
6	A	2602	UAF	C01-N02	2.54	1.50	1.46
5	D	2601	DG3	C6-N1	-2.39	1.34	1.38
5	A	2601	DG3	C6-N1	-2.37	1.34	1.38
6	A	2602	UAF	C08-N07	2.37	1.38	1.35
6	A	2602	UAF	C11-C12	2.34	1.51	1.43
5	A	2601	DG3	PB-O3A	2.04	1.61	1.59
5	D	2601	DG3	C5-N7	-2.00	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2601	DG3	C5-C4-N3	-6.11	118.67	128.39
5	D	2601	DG3	C5-C4-N3	-6.08	118.72	128.39
5	A	2601	DG3	C2-N3-C4	5.07	121.03	112.30
5	D	2601	DG3	C2-N3-C4	5.06	121.01	112.30
5	A	2601	DG3	N9-C4-N3	4.49	134.94	125.95
5	D	2601	DG3	N9-C4-N3	4.47	134.89	125.95
5	D	2601	DG3	C6-C5-N7	3.32	136.34	130.29
5	A	2601	DG3	C6-C5-N7	3.27	136.25	130.29
5	D	2601	DG3	C3'-C2'-C1'	2.79	106.09	102.87
6	A	2602	UAF	F17-C14-C13	2.69	116.81	112.40
6	A	2602	UAF	C23-C18-N02	2.63	123.49	120.08
5	A	2601	DG3	C3'-C2'-C1'	2.60	105.87	102.87
5	D	2601	DG3	C4-C5-N7	-2.60	106.56	110.67
5	A	2601	DG3	C4-C5-N7	-2.57	106.60	110.67
6	A	2602	UAF	C09-C10-C11	-2.44	105.70	109.27
6	A	2602	UAF	C10-C09-C08	-2.15	105.72	107.72
5	D	2601	DG3	O6-C6-C5	-2.09	121.03	126.53
5	A	2601	DG3	O6-C6-C5	-2.08	121.03	126.53
6	A	2602	UAF	F15-C14-C13	2.05	115.75	112.40
6	A	2602	UAF	C05-C03-S04	-2.01	116.67	120.11

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2601	DG3	C5'-O5'-PA-O3A
5	A	2601	DG3	C5'-O5'-PA-O1A
5	A	2601	DG3	C5'-O5'-PA-O2A
5	D	2601	DG3	C5'-O5'-PA-O3A
5	D	2601	DG3	C5'-O5'-PA-O1A

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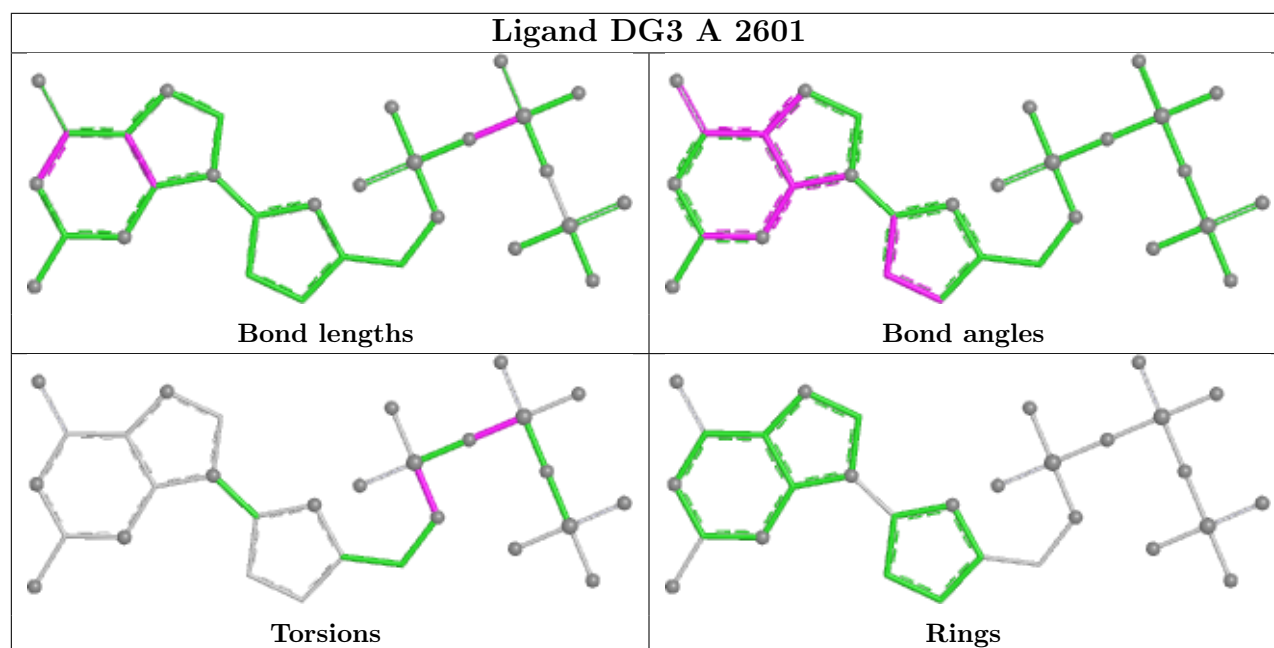
Mol	Chain	Res	Type	Atoms
5	D	2601	DG3	C5'-O5'-PA-O2A
6	A	2602	UAF	C03-C05-N06-N07
5	D	2601	DG3	PB-O3B-PG-O2G
5	A	2601	DG3	PA-O3A-PB-O2B
5	D	2601	DG3	PA-O3A-PB-O1B
5	A	2601	DG3	PA-O3A-PB-O1B
5	D	2601	DG3	PA-O3A-PB-O2B

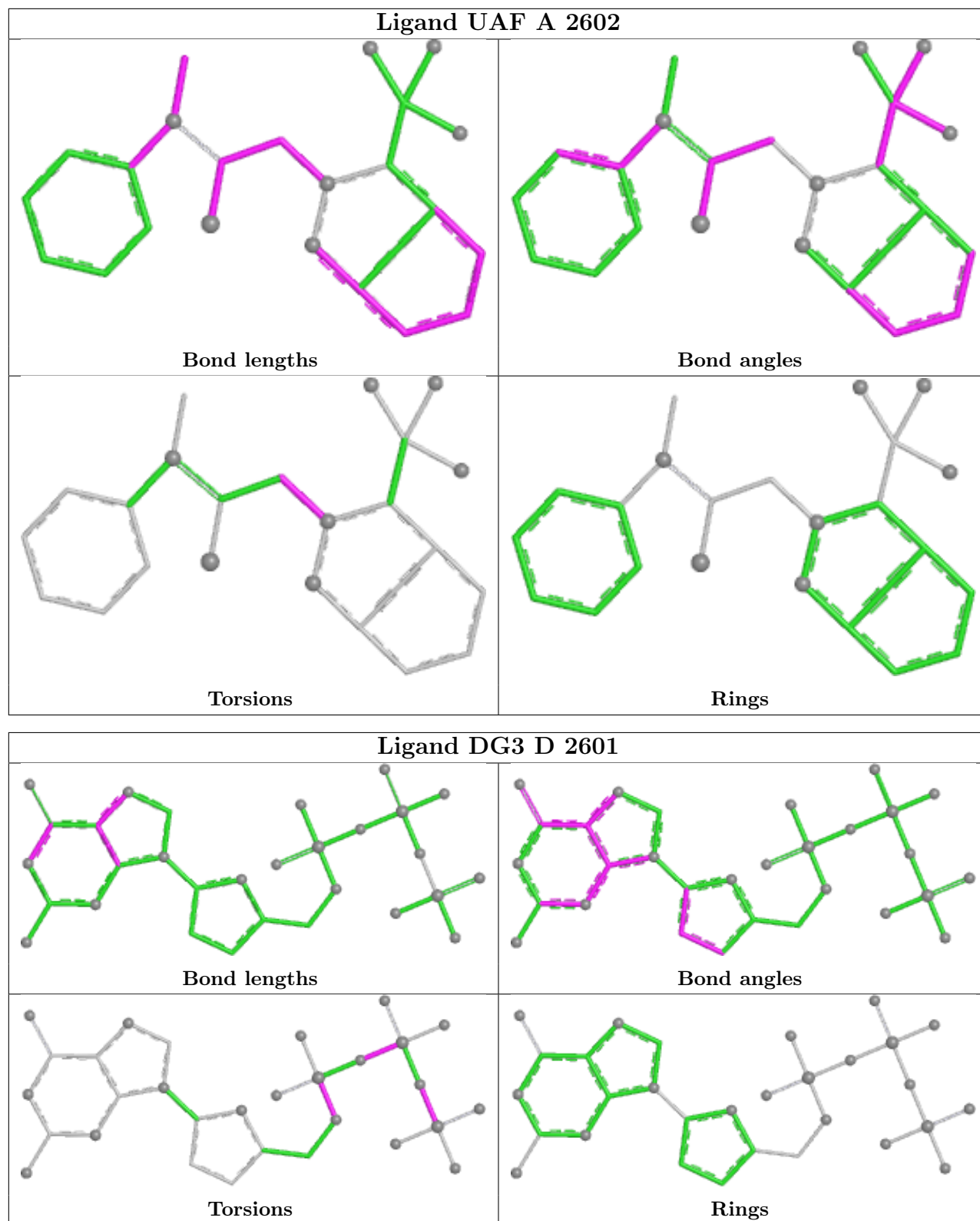
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2601	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/668 (95%)	0.67	48 (7%) 20 16	48, 77, 119, 187	0
1	D	603/668 (90%)	2.06	282 (46%) 0 0	66, 129, 187, 246	0
2	B	15/17 (88%)	0.44	0 100 100	63, 91, 200, 233	0
2	E	12/17 (70%)	0.52	0 100 100	99, 119, 171, 175	0
3	C	11/13 (84%)	0.67	1 (9%) 15 11	62, 125, 215, 217	0
3	F	8/13 (61%)	0.96	0 100 100	130, 136, 175, 186	0
All	All	1286/1396 (92%)	1.32	331 (25%) 1 1	48, 94, 177, 246	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2488	ILE	6.9
1	D	2318	PHE	6.9
1	D	2314	MET	6.8
1	D	2099	CYS	6.5
1	D	2345	ASP	6.5
1	D	2582	TRP	6.1
1	D	2210	VAL	6.0
1	D	2326	ILE	5.9
1	D	2224	LEU	5.8
1	D	2544	TYR	5.5
1	D	2317	ALA	5.5
1	D	2328	ALA	5.4
1	D	2402	MET	5.4
1	D	2469	ILE	5.4
1	D	2359	PHE	5.2
1	D	2386	CYS	5.0
1	D	2340	ALA	5.0
1	D	2527	CYS	5.0
1	D	2093	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	2362	ILE	4.9
1	D	2546	VAL	4.9
1	D	2249	ILE	4.9
1	D	2203	ILE	4.8
1	D	2312	ILE	4.8
1	D	2559	LYS	4.8
1	D	2348	LEU	4.7
1	D	2541	GLU	4.7
1	D	2416	PHE	4.7
1	D	2561	GLU	4.7
1	D	2325	SER	4.6
1	D	2530	ARG	4.6
1	D	2492	LEU	4.6
1	D	2212	PHE	4.5
1	D	2580	ALA	4.5
1	D	2548	GLU	4.5
1	D	2385	ILE	4.4
1	D	2565	ALA	4.4
1	D	2214	LEU	4.4
1	A	1896	ASP	4.3
1	D	2327	LEU	4.3
1	D	2535	ILE	4.3
1	D	2485	THR	4.3
1	D	2109	LYS	4.3
1	D	2413	ILE	4.2
1	D	2037	GLY	4.2
1	A	2031	SER	4.2
1	D	2401	GLN	4.2
1	D	2498	THR	4.1
1	A	2310	PHE	4.1
1	D	2489	GLN	4.1
1	A	1955	GLU	4.1
1	D	2422	GLY	4.1
1	D	2551	VAL	4.1
1	D	2223	PHE	4.1
1	A	2508	MET	4.0
1	D	2590	VAL	4.0
1	A	1958	LYS	4.0
1	D	2443	ILE	4.0
1	D	2142	LYS	4.0
1	D	2423	ILE	4.0
1	D	2193	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	2092	ILE	4.0
1	D	2391	TYR	4.0
1	A	2148	GLU	3.9
1	D	2024	GLU	3.9
1	D	2145	PRO	3.9
1	D	2500	LYS	3.9
1	D	2331	TYR	3.9
1	D	2534	PHE	3.9
1	D	2110	LEU	3.9
1	D	2256	PHE	3.8
1	D	2187	LEU	3.8
1	D	2439	PHE	3.8
1	D	2503	GLY	3.8
1	D	2229	ILE	3.8
1	D	2562	MET	3.7
1	A	2355	GLY	3.7
1	D	2378	LEU	3.7
1	D	2473	VAL	3.7
1	D	2112	ALA	3.7
1	D	2507	GLY	3.7
1	D	2105	ILE	3.7
1	A	2354	THR	3.7
1	D	2190	LEU	3.7
1	D	2376	ASP	3.7
1	D	2387	TYR	3.7
1	D	2198	LEU	3.6
1	D	2352	LEU	3.6
1	D	2226	MET	3.6
1	D	2420	TYR	3.6
1	D	2258	ILE	3.6
1	A	2353	ASN	3.6
1	D	2221	ASN	3.5
1	D	2403	GLY	3.5
1	D	2499	PHE	3.5
1	D	2208	THR	3.5
1	D	2334	LEU	3.5
1	D	2542	LEU	3.5
1	D	2316	HIS	3.5
1	D	2440	VAL	3.5
1	D	2411	CYS	3.5
1	D	2412	TYR	3.5
1	D	2313	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	2366	TRP	3.5
1	D	2484	ALA	3.4
1	D	2330	ASP	3.4
1	D	2239	THR	3.4
1	A	1864	SER	3.4
1	A	1865	SER	3.4
1	D	2358	VAL	3.4
1	D	2576	VAL	3.4
1	D	2113	ILE	3.4
1	D	2186	LYS	3.4
1	D	1859	ILE	3.4
1	D	2189	ALA	3.4
1	D	2390	ILE	3.4
1	D	1860	ARG	3.3
1	A	1846	CYS	3.3
1	D	2144	PRO	3.3
1	D	1920	GLU	3.3
1	D	2349	ILE	3.3
1	A	2025	THR	3.3
1	A	1824	SER	3.3
1	D	2426	PHE	3.3
1	D	2585	LEU	3.3
1	D	2480	ILE	3.3
1	A	2260	MET	3.2
1	D	2494	THR	3.2
1	D	2478	ALA	3.2
1	D	2101	SER	3.2
1	D	1935	LEU	3.2
1	D	2336	LEU	3.2
1	D	2557	ILE	3.2
1	D	2380	GLN	3.2
1	D	2255	ASP	3.2
1	D	2222	PRO	3.2
1	D	2371	PRO	3.2
1	D	2205	ASN	3.2
1	D	2253	PRO	3.1
1	A	2507	GLY	3.1
1	D	2091	GLY	3.1
1	D	2315	ARG	3.1
1	D	2215	GLN	3.1
1	D	2588	PHE	3.1
1	A	2495	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	2538	LEU	3.1
1	A	2590	VAL	3.1
1	D	2536	LEU	3.1
1	D	2572	LEU	3.0
1	A	2147	ARG	3.0
1	D	2583	GLY	3.0
1	D	2558	VAL	3.0
1	D	2442	THR	3.0
1	D	1934	SER	3.0
1	D	2417	LYS	3.0
1	D	2428	THR	3.0
1	D	2322	PRO	3.0
1	D	2444	LEU	3.0
1	D	2476	SER	3.0
1	D	2424	ASN	3.0
1	D	2502	HIS	3.0
1	D	2540	ASP	3.0
1	D	2581	SER	3.0
1	D	2102	GLN	3.0
1	D	2389	ILE	2.9
1	D	2539	HIS	2.9
1	A	1838	GLN	2.9
1	D	2491	GLN	2.9
1	D	2483	ILE	2.9
1	A	2498	THR	2.9
1	A	2029	ILE	2.9
1	D	2133	ILE	2.9
1	D	2219	CYS	2.9
1	D	2586	LYS	2.9
1	D	2137	LEU	2.9
1	A	2499	PHE	2.9
1	D	2578	ILE	2.9
1	D	2115	THR	2.9
1	D	2247	PRO	2.9
1	D	1976	LEU	2.9
1	D	1965	TYR	2.9
1	A	2332	SER	2.8
1	D	2207	ILE	2.8
1	D	2107	GLN	2.8
1	D	2347	ARG	2.8
1	D	2343	SER	2.8
1	D	2183	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	2446	ARG	2.8
1	D	2248	ASN	2.8
1	D	1919	LYS	2.8
1	A	2407	ASN	2.7
1	A	2458	PRO	2.7
1	A	2497	SER	2.7
1	D	2566	VAL	2.7
1	D	2574	VAL	2.7
1	D	2086	LEU	2.7
1	D	2108	ALA	2.7
1	D	2250	GLN	2.7
1	D	2552	VAL	2.7
1	D	2196	LEU	2.7
1	D	2209	LYS	2.7
1	D	2329	ALA	2.7
1	D	2421	THR	2.7
1	D	2227	GLU	2.7
1	D	2404	ILE	2.7
1	D	1821	SER	2.7
1	D	2127	PHE	2.7
1	D	2211	VAL	2.7
1	D	2228	ARG	2.7
1	D	2543	LEU	2.7
1	D	2550	ASP	2.6
1	D	2073	PHE	2.6
1	D	2177	PHE	2.6
1	D	2252	VAL	2.6
1	D	2342	LEU	2.6
1	A	2363	ALA	2.6
1	D	2468	ALA	2.6
1	D	2123	HIS	2.6
1	D	2367	LYS	2.6
1	D	2213	PRO	2.6
1	D	2231	PRO	2.6
1	D	2545	GLU	2.6
1	D	1898	THR	2.6
1	D	2075	LYS	2.6
1	D	2023	MET	2.6
1	D	2141	LEU	2.6
1	D	2350	GLN	2.6
1	A	2356	ALA	2.6
1	D	2216	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1936	ASP	2.5
1	D	2192	PRO	2.5
1	D	2493	GLU	2.5
1	D	2351	VAL	2.5
1	D	2374	VAL	2.5
1	D	2486	VAL	2.5
1	D	2529	ILE	2.5
1	D	2563	GLU	2.5
1	D	1939	LEU	2.5
1	D	2234	GLN	2.5
1	A	1825	LEU	2.5
1	A	1899	LEU	2.5
1	D	2120	LEU	2.5
1	D	2121	ALA	2.5
1	D	2429	GLU	2.5
1	D	2475	GLY	2.5
1	D	2408	ASP	2.5
1	D	2474	GLN	2.5
1	D	2382	ALA	2.5
1	A	2023	MET	2.5
1	D	2394	GLY	2.4
1	D	2577	LYS	2.4
1	D	2089	LEU	2.4
1	D	2083	CYS	2.4
1	D	2490	LYS	2.4
1	D	2579	GLY	2.4
1	D	2414	ASP	2.4
1	D	2044	TYR	2.4
1	D	1850	PHE	2.4
1	D	2369	ILE	2.4
1	D	2344	HIS	2.4
1	D	2471	THR	2.4
1	A	2570	VAL	2.4
1	D	2570	VAL	2.4
3	C	3	DG	2.4
1	A	2182	ASP	2.3
1	A	2589	ASP	2.3
1	D	2341	HIS	2.3
1	D	2206	ALA	2.3
1	D	2217	GLU	2.3
1	D	2035	ASN	2.3
1	D	2184	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	2479	ASP	2.3
1	D	1958	LYS	2.3
1	D	2125	PHE	2.3
1	D	2375	GLY	2.3
1	A	2026	SER	2.3
1	D	2501	SER	2.3
1	A	2019	LEU	2.3
1	D	2240	GLY	2.2
1	D	2355	GLY	2.2
1	A	1935	LEU	2.2
1	A	2017	LEU	2.2
1	D	2087	LEU	2.2
1	D	2398	LEU	2.2
1	D	2135	GLU	2.2
1	D	2553	GLN	2.2
1	D	2584	GLU	2.2
1	D	2036	ALA	2.2
1	D	2251	ASN	2.2
1	D	2333	GLN	2.2
1	D	2230	TYR	2.2
1	D	2323	GLY	2.2
1	A	1828	ILE	2.2
1	D	2029	ILE	2.2
1	D	2379	ARG	2.2
1	D	2103	LYS	2.2
1	A	2027	GLN	2.1
1	D	1908	GLY	2.1
1	D	2020	LEU	2.1
1	D	2245	THR	2.1
1	A	2529	ILE	2.1
1	D	1949	GLN	2.1
1	D	2393	MET	2.1
1	D	2117	ALA	2.1
1	D	2346	ARG	2.1
1	D	2357	ASP	2.1
1	A	2015	HIS	2.1
1	D	2356	ALA	2.1
1	D	2410	ALA	2.1
1	D	2002	GLU	2.1
1	D	2199	GLU	2.1
1	D	2335	GLU	2.1
1	D	2427	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2136	VAL	2.1
1	D	2200	TRP	2.1
1	D	2202	ARG	2.1
1	D	2106	MET	2.1
1	D	2587	ASP	2.0
1	A	1950	SER	2.0
1	D	2368	MET	2.0
1	A	2177	PHE	2.0
1	A	2183	VAL	2.0
1	D	1899	LEU	2.0
1	D	2143	LEU	2.0
1	D	2220	LEU	2.0
1	D	2560	ASN	2.0
1	A	2369	ILE	2.0
1	D	2354	THR	2.0
1	D	2453	ILE	2.0
1	D	2178	SER	2.0
1	D	2361	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

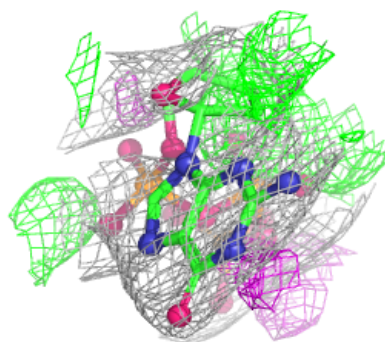
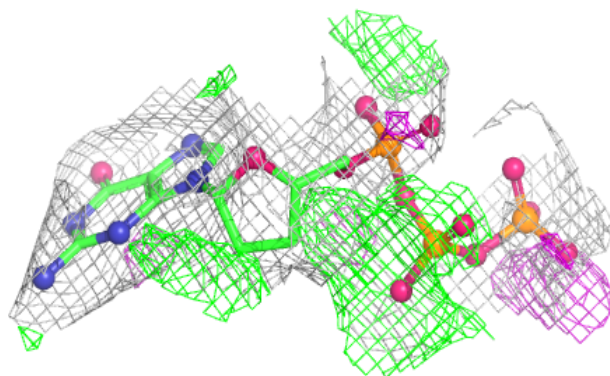
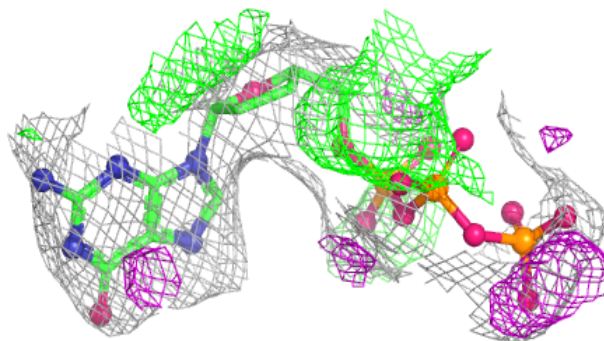
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DG3	D	2601	30/30	0.70	0.16	109,138,158,164	0
4	MG	D	2600	1/1	0.76	0.12	146,146,146,146	0
6	UAF	A	2602	23/23	0.95	0.12	58,70,78,82	0
4	MG	A	2600	1/1	0.96	0.06	62,62,62,62	0
5	DG3	A	2601	30/30	0.97	0.08	47,63,78,84	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.

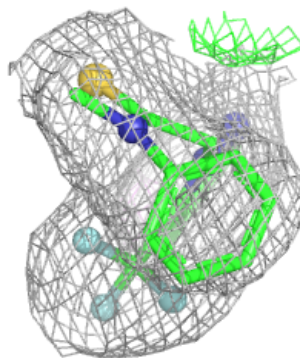
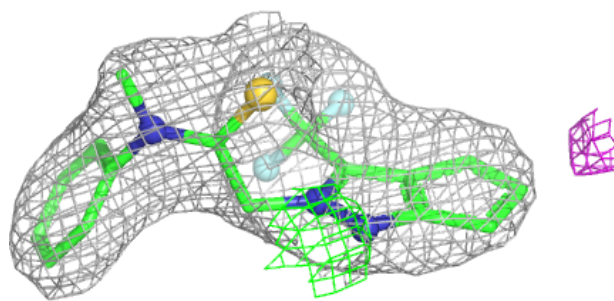
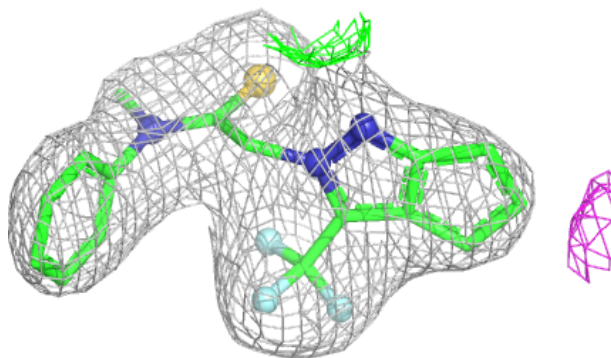
Electron density around DG3 D 2601:

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

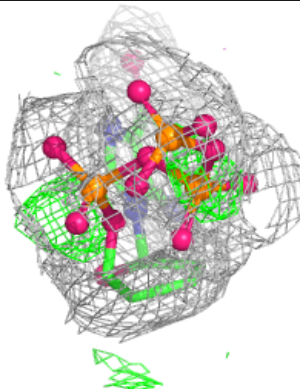
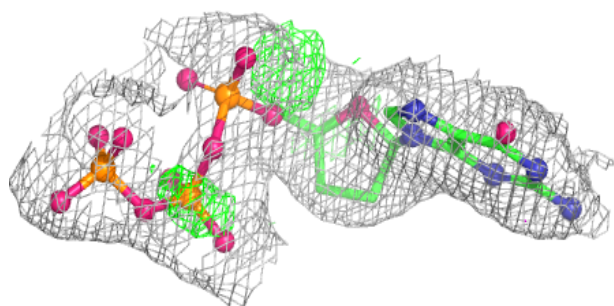
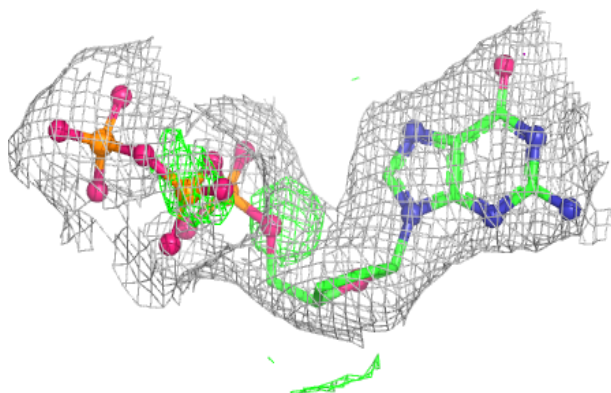


Electron density around UAF A 2602:

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

**Electron density around DG3 A 2601:**

$2mF_o-DF_c$ (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.