



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 06:50 PM UTC

PDB ID : 7ZUS / pdb_00007zus
Title : Crystal structure of ternary complex of Pol theta polymerase domain
Authors : Krajewski, W.W.; Turnbull, A.P.; Willis, S.; Charles, M.; Stockley, M.; Heald, R.A.
Deposited on : 2022-05-13
Resolution : 2.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

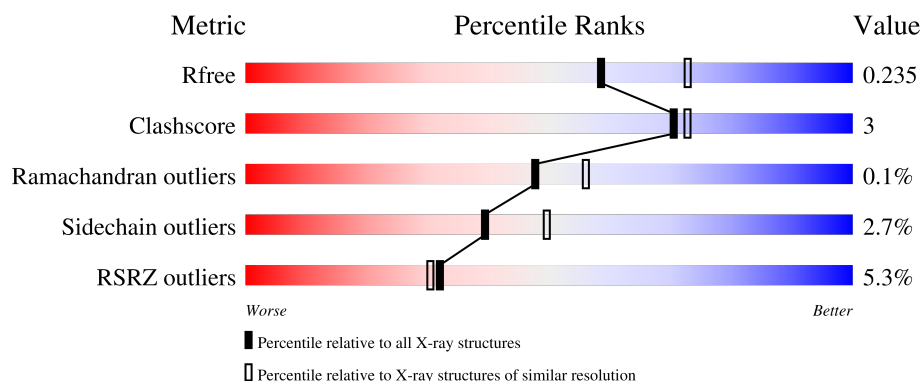
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	AAA	726	5% 79% 9% 12%
1	BBB	726	4% 79% 8% 12%
1	CCC	726	6% 81% 8% 10%
2	DDD	16	81% 6% 12%
2	FFF	16	81% 12% 6%

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Mol	Chain	Length	Quality of chain
2	HHH	16	 88% 12%
3	EEE	13	 62% 31% 8%
3	GGG	13	 85% 15%
3	III	13	 69% 31%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16842 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	AAA	639	Total	C	N	O	S	0	0	0
			4882	3125	825	903	29			
1	BBB	639	Total	C	N	O	S	0	0	0
			4898	3135	828	905	30			
1	CCC	650	Total	C	N	O	S	0	0	0
			4937	3153	832	924	28			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2261	GLY	PRO	engineered mutation	UNP O75417
AAA	?	-	THR	deletion	UNP O75417
AAA	?	-	LEU	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	LEU	deletion	UNP O75417
AAA	?	-	LEU	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	MET	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	TYR	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	LYS	deletion	UNP O75417
AAA	?	-	GLY	deletion	UNP O75417
AAA	?	-	PHE	deletion	UNP O75417
AAA	?	-	SER	deletion	UNP O75417
AAA	?	-	VAL	deletion	UNP O75417
AAA	?	-	ASN	deletion	UNP O75417
AAA	?	-	PRO	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	CYS	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	GLN	deletion	UNP O75417
AAA	?	-	MET	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	GLU	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	ALA	deletion	UNP O75417
AAA	?	-	ASP	deletion	UNP O75417
AAA	?	-	ARG	deletion	UNP O75417
BBB	2261	GLY	PRO	engineered mutation	UNP O75417
BBB	?	-	THR	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	LEU	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	MET	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	TYR	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	LYS	deletion	UNP O75417
BBB	?	-	GLY	deletion	UNP O75417
BBB	?	-	PHE	deletion	UNP O75417
BBB	?	-	SER	deletion	UNP O75417
BBB	?	-	VAL	deletion	UNP O75417
BBB	?	-	ASN	deletion	UNP O75417
BBB	?	-	PRO	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	CYS	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	GLN	deletion	UNP O75417
BBB	?	-	MET	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	GLU	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	ALA	deletion	UNP O75417
BBB	?	-	ASP	deletion	UNP O75417
BBB	?	-	ARG	deletion	UNP O75417
CCC	2261	GLY	PRO	engineered mutation	UNP O75417
CCC	?	-	THR	deletion	UNP O75417
CCC	?	-	LEU	deletion	UNP O75417
CCC	?	-	VAL	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	GLU	deletion	UNP O75417
CCC	?	-	SER	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417
CCC	?	-	PRO	deletion	UNP O75417
CCC	?	-	SER	deletion	UNP O75417
CCC	?	-	GLN	deletion	UNP O75417
CCC	?	-	ALA	deletion	UNP O75417
CCC	?	-	VAL	deletion	UNP O75417
CCC	?	-	GLY	deletion	UNP O75417
CCC	?	-	LYS	deletion	UNP O75417

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DDD	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	FFF	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			
2	HHH	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			

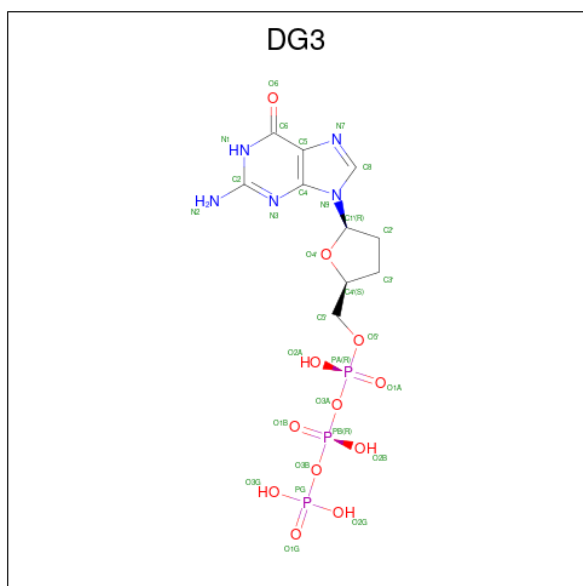
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EEE	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	GGG	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
3	III	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		
4	BBB	1	Total	Mg	0	0
			1	1		
4	CCC	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

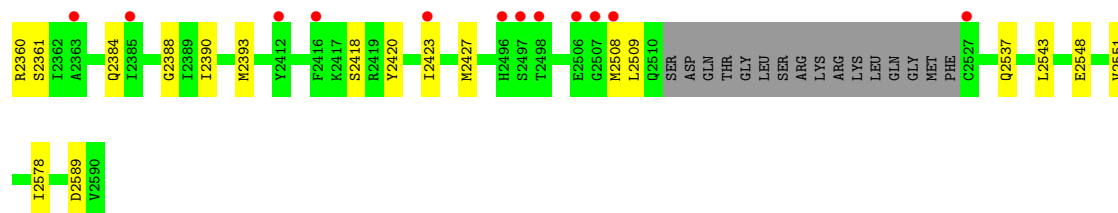
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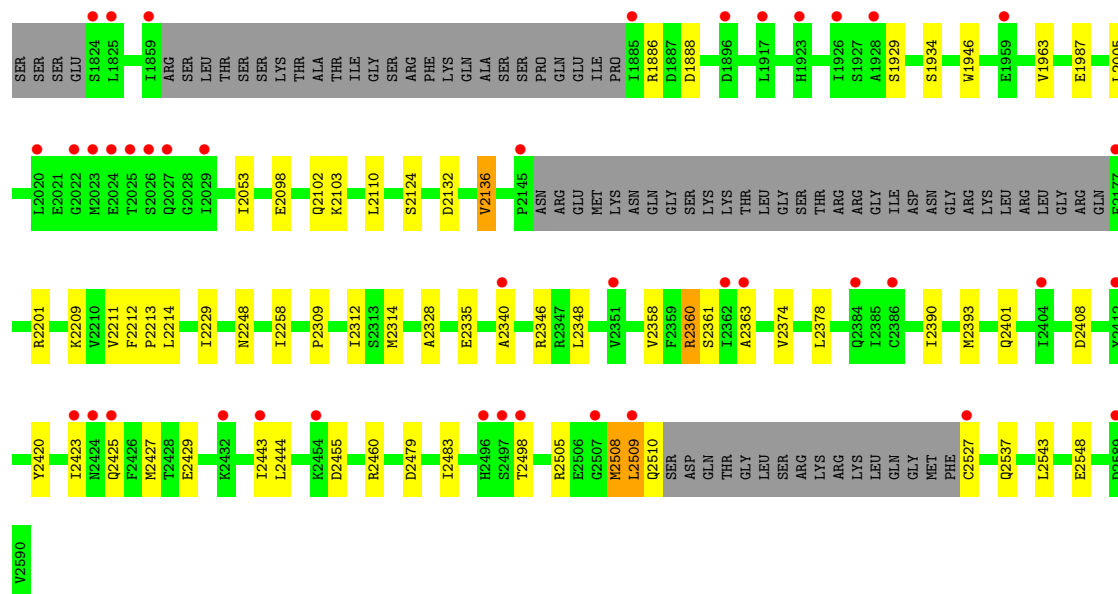
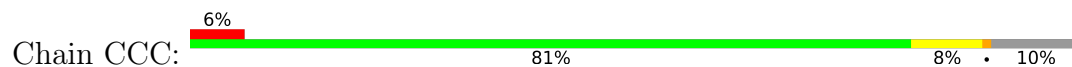
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	CCC	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is water.

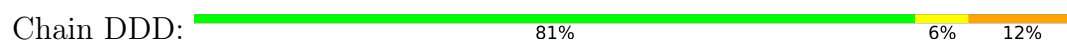
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	116	Total	O	0	0
			116	116		
6	BBB	71	Total	O	0	0
			71	71		
6	CCC	44	Total	O	0	0
			44	44		
6	DDD	6	Total	O	0	0
			6	6		
6	EEE	4	Total	O	0	0
			4	4		
6	FFF	4	Total	O	0	0
			4	4		
6	GGG	9	Total	O	0	0
			9	9		
6	HHH	10	Total	O	0	0
			10	10		
6	III	4	Total	O	0	0
			4	4		



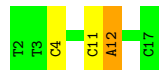
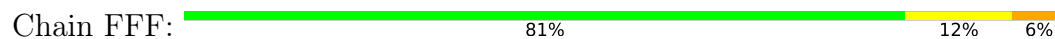
- Molecule 1: DNA polymerase theta



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



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



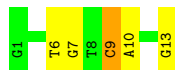
- Molecule 2: DNA (5'-D(P*TP*TP*CP*CP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*C)-3')





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

Chain EEE:  62% 31% 8%



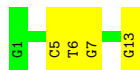
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*(DDG))-3')

Chain GGG:  85% 15%



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

Chain III:  69% 31%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	288.81Å 172.91Å 58.75Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	50.01 – 2.26 50.01 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.01-2.26) 98.9 (50.01-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.238 0.202 , 0.235	Depositor DCC
R_{free} test set	6681 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.009 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.028 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.023 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16842	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DDG, DG3, 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	AAA	1.12	6/4978 (0.1%)	1.46	8/6748 (0.1%)
1	BBB	1.09	2/4994 (0.0%)	1.43	2/6766 (0.0%)
1	CCC	1.06	1/5033 (0.0%)	1.43	0/6829
2	DDD	0.78	0/362	1.19	3/555 (0.5%)
2	FFF	0.78	0/362	1.10	1/555 (0.2%)
2	HHH	0.77	0/362	1.08	1/555 (0.2%)
3	EEE	0.83	0/271	1.31	3/417 (0.7%)
3	GGG	0.82	0/271	1.18	1/417 (0.2%)
3	III	0.78	0/271	1.21	1/417 (0.2%)
All	All	1.06	9/16904 (0.1%)	1.41	20/23259 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	2003	PRO	C-O	-6.94	1.16	1.23
1	AAA	2236	HIS	CE1-NE2	5.83	1.38	1.32
1	AAA	1986	TYR	C-O	5.52	1.30	1.24
1	BBB	1946	TRP	C-O	5.43	1.30	1.24
1	AAA	1989	PRO	C-O	-5.18	1.17	1.24

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	III	7	DG	P-O3'-C3'	-10.55	104.38	120.20
3	GGG	7	DG	P-O3'-C3'	-10.02	105.18	120.20
3	EEE	7	DG	P-O3'-C3'	-9.43	106.06	120.20
3	EEE	9	DC	P-O3'-C3'	-8.41	107.58	120.20
2	DDD	11	DC	O3'-P-O5'	-7.14	93.29	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4882	0	4712	31	0
1	BBB	4898	0	4741	36	0
1	CCC	4937	0	4734	38	0
2	DDD	324	0	180	1	0
2	FFF	324	0	180	4	0
2	HHH	324	0	180	1	0
3	EEE	264	0	149	1	0
3	GGG	264	0	149	0	0
3	III	264	0	149	1	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	30	0	12	0	0
5	BBB	30	0	12	0	0
5	CCC	30	0	12	1	0
6	AAA	116	0	0	1	0
6	BBB	71	0	0	0	0
6	CCC	44	0	0	2	0
6	DDD	6	0	0	0	0
6	EEE	4	0	0	0	0
6	FFF	4	0	0	0	0
6	GGG	9	0	0	0	0
6	HHH	10	0	0	0	0
6	III	4	0	0	0	0
All	All	16842	0	15210	107	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 3.

The worst 5 of 107 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:BBB:2023:MET:HE1	1:BBB:2048:VAL:HG11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:2340:ALA:HB2	1:BBB:2348:LEU:HD22	1.67	0.75
1:AAA:2496:HIS:CG	1:AAA:2498:THR:O	2.40	0.75
1:CCC:2340:ALA:HB2	1:CCC:2348:LEU:HD22	1.69	0.74
1:BBB:2019:LEU:O	1:BBB:2023:MET:HE2	1.90	0.72

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	AAA	629/726 (87%)	612 (97%)	16 (2%)	1 (0%)	43	50
1	BBB	629/726 (87%)	615 (98%)	14 (2%)	0	100	100
1	CCC	642/726 (88%)	627 (98%)	14 (2%)	1 (0%)	43	50
All	All	1900/2178 (87%)	1854 (98%)	44 (2%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	2356	ALA
1	CCC	2498	THR

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	AAA	499/638 (78%)	486 (97%)	13 (3%)	40	50
1	BBB	502/638 (79%)	488 (97%)	14 (3%)	38	48
1	CCC	503/638 (79%)	489 (97%)	14 (3%)	38	48
All	All	1504/1914 (79%)	1463 (97%)	41 (3%)	39	49

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	1934	SER
1	CCC	2361	SER
1	CCC	2124	SER
1	CCC	2346	ARG
1	CCC	2508	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DDG	III	13	3,2	20,23,24	1.51	2 (10%)	27,33,36	2.49	13 (48%)
3	DDG	EEE	13	3,2	20,23,24	1.70	4 (20%)	27,33,36	2.59	12 (44%)
3	DDG	GGG	13	3,2	20,23,24	1.39	2 (10%)	27,33,36	2.71	14 (51%)

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
3	DDG	III	13	3,2	-	0/7/18/19	0/3/3/3
3	DDG	EEE	13	3,2	-	0/7/18/19	0/3/3/3
3	DDG	GGG	13	3,2	-	0/7/18/19	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	EEE	13	DDG	C5-N7	-4.15	1.30	1.39
3	III	13	DDG	C5-N7	-4.12	1.30	1.39
3	GGG	13	DDG	C5-N7	-3.64	1.31	1.39
3	EEE	13	DDG	C5-C4	3.56	1.48	1.38
3	III	13	DDG	C5-C4	3.45	1.48	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EEE	13	DDG	C5-C4-N3	-5.95	118.92	128.39
3	GGG	13	DDG	C2-N3-C4	5.88	122.42	112.30
3	EEE	13	DDG	C2-N3-C4	5.85	122.38	112.30
3	III	13	DDG	C5-C4-N3	-5.84	119.10	128.39
3	GGG	13	DDG	C5-C4-N3	-5.64	119.41	128.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 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	AAA	2602	4	31,32,32	0.62	0	44,50,50	0.90	2 (4%)
5	DG3	BBB	2602	4	31,32,32	0.64	0	44,50,50	0.75	0
5	DG3	CCC	2602	4	31,32,32	0.61	0	44,50,50	0.77	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
5	DG3	AAA	2602	4	-	3/22/31/31	0/3/3/3
5	DG3	BBB	2602	4	-	5/22/31/31	0/3/3/3
5	DG3	CCC	2602	4	-	6/22/31/31	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	2602	DG3	O2G-PG-O3B	2.48	112.96	104.64
5	AAA	2602	DG3	O3B-PG-O1G	-2.02	100.42	111.04

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

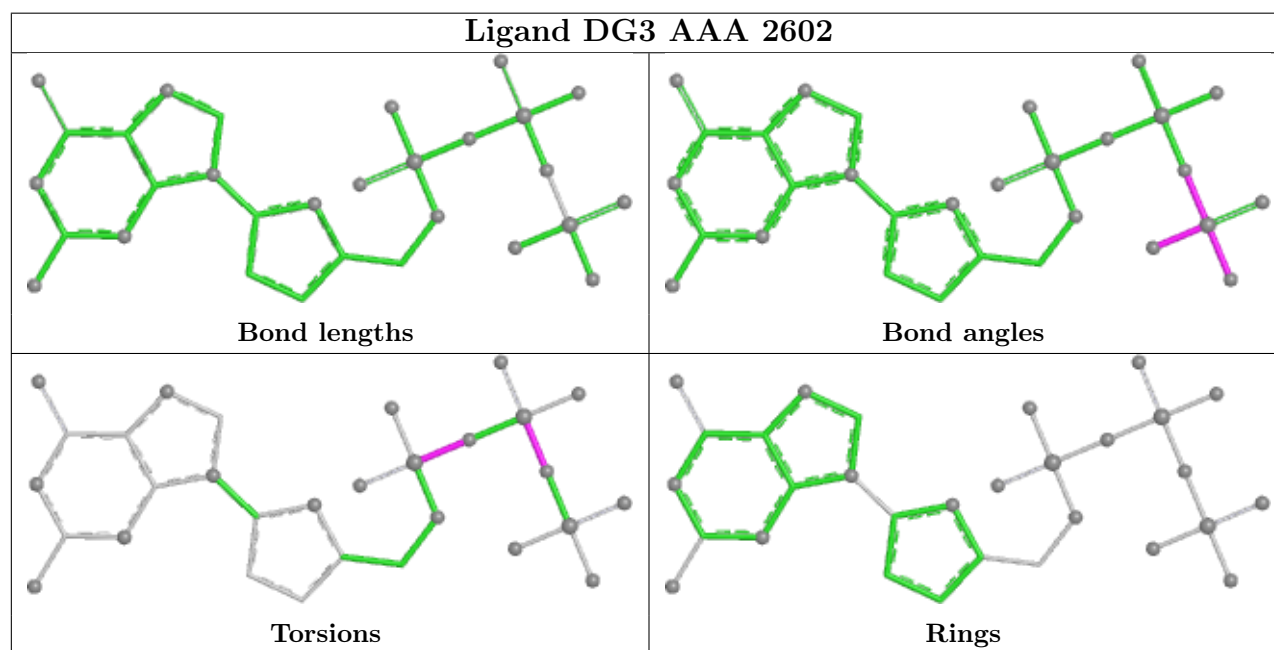
Mol	Chain	Res	Type	Atoms
5	BBB	2602	DG3	PB-O3B-PG-O2G
5	CCC	2602	DG3	PB-O3B-PG-O2G
5	AAA	2602	DG3	PG-O3B-PB-O2B
5	CCC	2602	DG3	PG-O3B-PB-O2B
5	AAA	2602	DG3	PB-O3A-PA-O2A

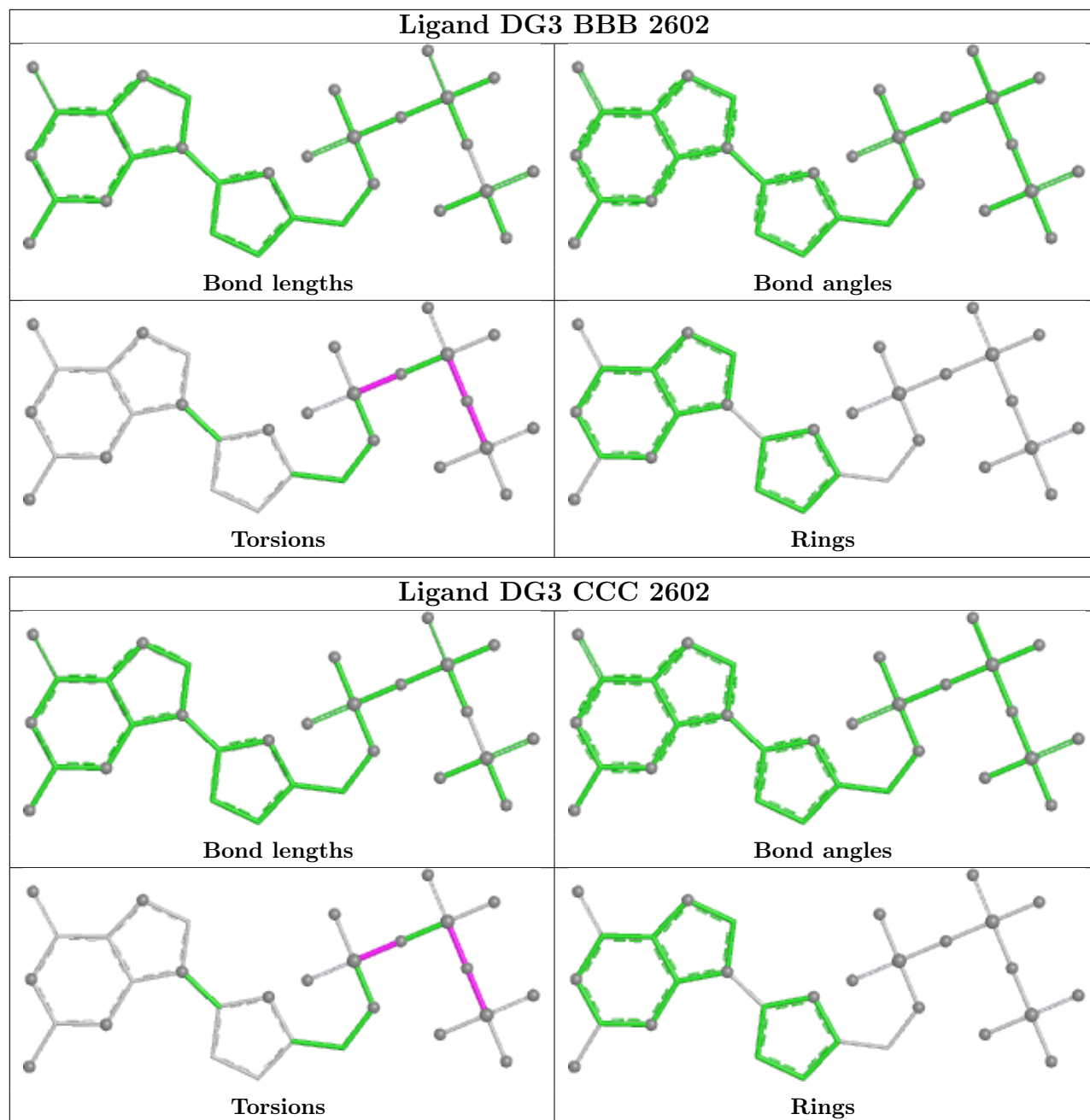
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	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.





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	AAA	639/726 (88%)	0.29	33 (5%)	33	31	38, 65, 113, 142	0
1	BBB	639/726 (88%)	0.45	32 (5%)	34	33	44, 72, 112, 132	0
1	CCC	650/726 (89%)	0.61	41 (6%)	26	24	48, 84, 121, 143	0
2	DDD	16/16 (100%)	0.10	0	100	100	49, 99, 173, 183	0
2	FFF	16/16 (100%)	-0.22	0	100	100	48, 80, 157, 165	0
2	HHH	16/16 (100%)	-0.25	0	100	100	55, 92, 147, 151	0
3	EEE	12/13 (92%)	0.19	0	100	100	50, 110, 155, 160	0
3	GGG	12/13 (92%)	-0.09	0	100	100	50, 102, 142, 146	0
3	III	12/13 (92%)	0.05	0	100	100	53, 105, 147, 151	0
All	All	2012/2265 (88%)	0.43	106 (5%)	32	30	38, 75, 119, 183	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	1859	ILE	5.0
1	AAA	2177	PHE	4.4
1	CCC	1859	ILE	4.4
1	CCC	1824	SER	4.4
1	BBB	2363	ALA	4.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DDG	EEE	13	21/22	0.97	0.06	45,48,53,56	0
3	DDG	III	13	21/22	0.97	0.06	50,52,59,63	0
3	DDG	GGG	13	21/22	0.98	0.06	45,49,55,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

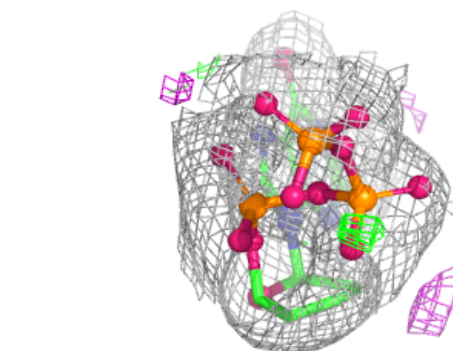
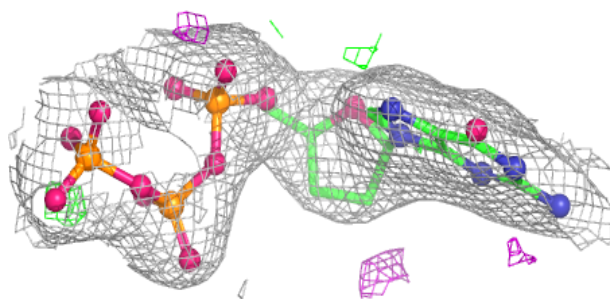
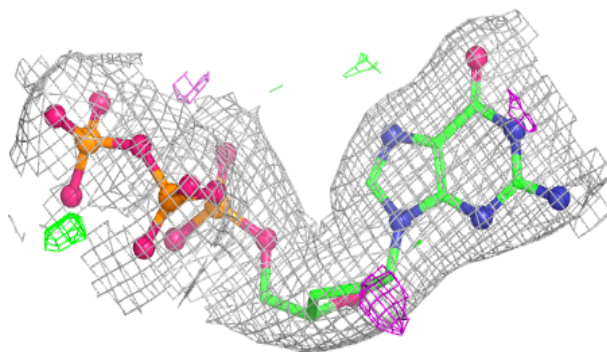
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DG3	CCC	2602	30/30	0.96	0.07	48,55,65,68	0
5	DG3	BBB	2602	30/30	0.97	0.06	48,56,63,68	0
4	MG	CCC	2601	1/1	0.98	0.06	63,63,63,63	0
5	DG3	AAA	2602	30/30	0.98	0.05	41,48,60,65	0
4	MG	AAA	2601	1/1	0.98	0.05	55,55,55,55	0
4	MG	BBB	2601	1/1	0.98	0.06	64,64,64,64	0

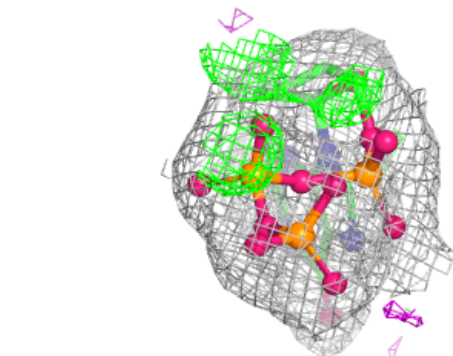
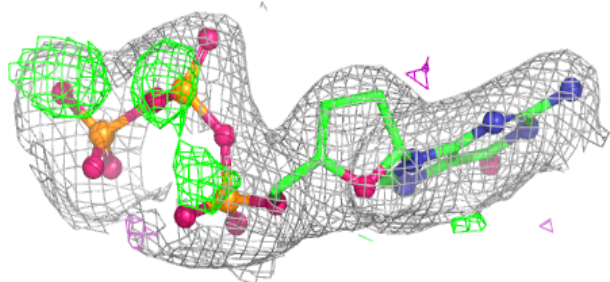
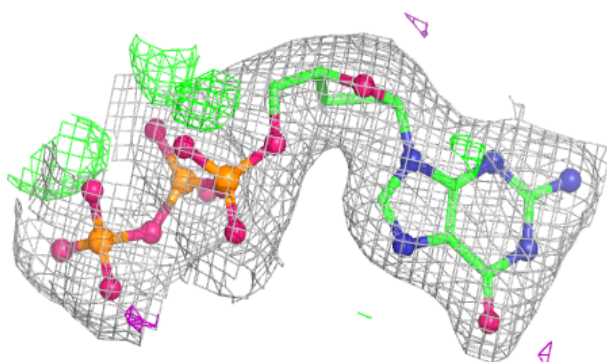
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DG3 CCC 2602:

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

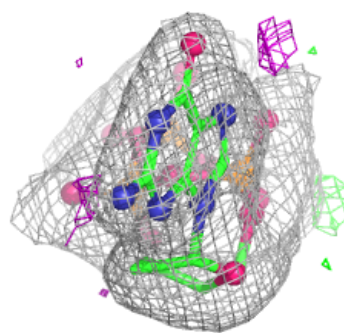
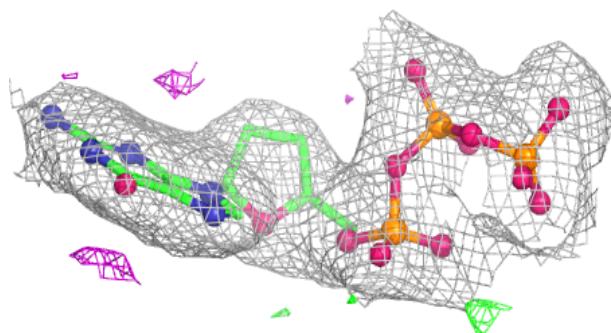
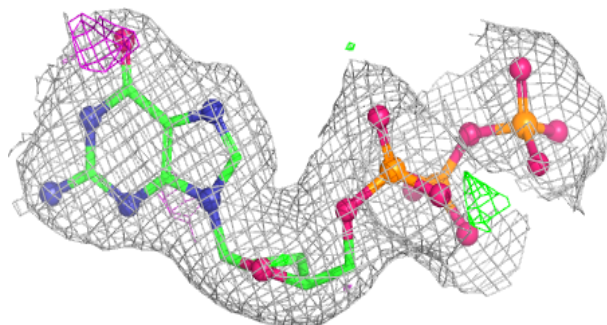
**Electron density around DG3 BBB 2602:**

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



Electron density around DG3 AAA 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.