



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 09:26 AM EDT

PDB ID : 8VAX / pdb_00008vax
Title : Cadmium catalyzed primer extension product with 14mer primer and mixed phosphorothioate activated G monomer
Authors : Fang, Z.; Szostak, J.W.
Deposited on : 2023-12-11
Resolution : 1.42 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

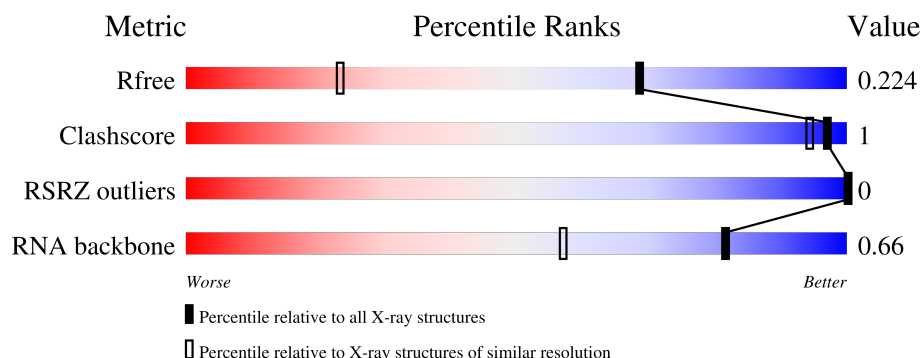
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)
RNA backbone	3983	1019 (2.10-0.86)

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	15	
1	BBB	15	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 878 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.

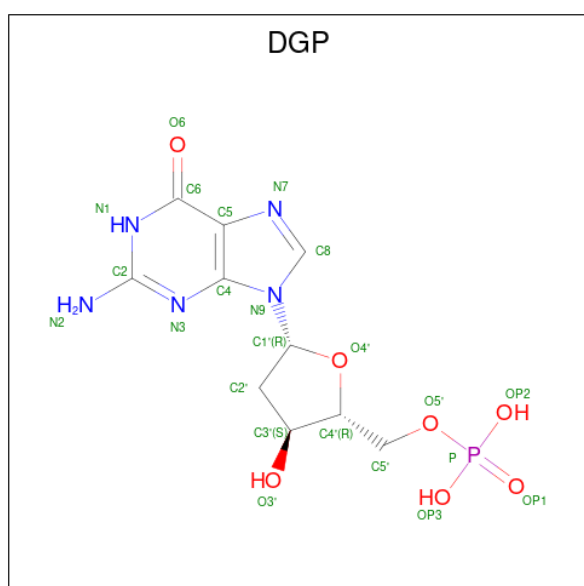
- Molecule 1 is a RNA chain called Cadmium catalyzed nonenzymatic RNA primer extension product.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	15	Total	C	N	O	P	S	0	0	0
			322	149	56	102	14	1			
1	BBB	15	Total	C	N	O	P	S	0	0	0
			322	149	56	102	14	1			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Mg	0	0
			2	2		
2	BBB	3	Total	Mg	0	0
			3	3		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (CCD ID: DGP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	BBB	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	BBB	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

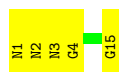
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	90	Total	O	0	0
			90	90		
4	BBB	93	Total	O	0	0
			93	93		

3 Residue-property plots

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: Cadmium catalyzed nonenzymatic RNA primer extension product

Chain AAA: 



- Molecule 1: Cadmium catalyzed nonenzymatic RNA primer extension product

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	43.47Å 43.47Å 83.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.94 – 1.42 41.94 – 1.42	Depositor EDS
% Data completeness (in resolution range)	90.2 (41.94-1.42) 90.2 (41.94-1.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.175 , 0.218 0.180 , 0.224	Depositor DCC
R_{free} test set	841 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	878	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0737e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DGP, LCG, LCC, MG, G46

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	0.68	0/236	1.15	0/365
1	BBB	0.68	0/236	1.10	2/365 (0.5%)
All	All	0.68	0/472	1.13	2/730 (0.3%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	10	A	O3'-P-O5'	-6.21	94.69	104.00
1	BBB	10	A	C4'-C3'-O3'	-5.47	104.80	113.00

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	AAA	322	0	170	0	0
1	BBB	322	0	170	1	0
2	AAA	2	0	0	0	0
2	BBB	3	0	0	0	0
3	BBB	46	0	24	0	0
4	AAA	90	0	0	0	1
4	BBB	93	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	878	0	364	1	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 1.

All (1) 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:6:C:OP2	4:BBB:201:HOH:O	2.03	0.75

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)
4:AAA:206:HOH:O	4:AAA:209:HOH:O[3_555]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AAA	14/15 (93%)	0	0
1	BBB	14/15 (93%)	0	0
All	All	28/30 (93%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

10 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
1	G46	BBB	15	1	21,25,26	1.29	3 (14%)	32,37,40	1.55	4 (12%)
1	LCC	AAA	1	1	21,21,25	2.69	5 (23%)	31,33,40	1.78	8 (25%)
1	LCG	AAA	4	1	24,27,28	1.51	2 (8%)	35,42,45	1.33	6 (17%)
1	LCC	AAA	2	1	21,24,25	2.35	10 (47%)	29,37,40	1.27	4 (13%)
1	LCG	BBB	4	1	24,27,28	1.33	3 (12%)	35,42,45	1.08	1 (2%)
1	LCC	BBB	2	1	21,24,25	2.19	7 (33%)	29,37,40	1.78	5 (17%)
1	LCC	BBB	3	1	21,24,25	2.23	8 (38%)	29,37,40	1.62	5 (17%)
1	LCC	AAA	3	1	21,24,25	1.96	5 (23%)	29,37,40	1.11	1 (3%)
1	G46	AAA	15	1	21,25,26	1.30	2 (9%)	32,37,40	1.72	9 (28%)
1	LCC	BBB	1	1	21,21,25	2.18	7 (33%)	31,33,40	2.03	8 (25%)

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
1	G46	BBB	15	1	-	0/7/25/26	0/3/3/3
1	LCC	AAA	1	1	-	0/7/32/36	0/4/3/3
1	LCG	AAA	4	1	-	0/8/35/36	0/5/4/4
1	LCC	AAA	2	1	-	0/8/35/36	0/4/3/3
1	LCG	BBB	4	1	-	0/8/35/36	0/5/4/4
1	LCC	BBB	2	1	-	0/8/35/36	0/4/3/3
1	LCC	BBB	3	1	-	0/8/35/36	0/4/3/3
1	LCC	AAA	3	1	-	0/8/35/36	0/4/3/3
1	G46	AAA	15	1	-	0/7/25/26	0/3/3/3
1	LCC	BBB	1	1	-	0/7/32/36	0/4/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	1	LCC	C5-C4	-7.37	1.38	1.44
1	AAA	1	LCC	O2'-C6'	7.07	1.55	1.43
1	AAA	2	LCC	C5-C4	-5.88	1.39	1.44
1	BBB	1	LCC	C5-C4	-5.35	1.40	1.44
1	AAA	3	LCC	O2'-C6'	5.28	1.52	1.43
1	BBB	3	LCC	C5-C4	-5.00	1.40	1.44
1	BBB	3	LCC	C4'-C3'	-4.87	1.48	1.53
1	BBB	2	LCC	O2'-C6'	4.69	1.51	1.43
1	BBB	2	LCC	O4'-C4'	-4.50	1.39	1.45
1	AAA	3	LCC	C4'-C3'	-4.02	1.49	1.53
1	BBB	3	LCC	C5M-C5	-3.78	1.41	1.50
1	AAA	1	LCC	C5M-C5	-3.69	1.41	1.50
1	AAA	2	LCC	O4'-C4'	-3.63	1.40	1.45
1	BBB	1	LCC	O2'-C6'	3.56	1.49	1.43
1	BBB	1	LCC	C5M-C5	-3.51	1.42	1.50
1	AAA	4	LCG	C4'-C3'	-3.51	1.49	1.53
1	BBB	2	LCC	C5M-C5	-3.42	1.42	1.50
1	AAA	4	LCG	O2'-C6'	3.28	1.49	1.43
1	BBB	2	LCC	C5-C4	-3.24	1.41	1.44
1	AAA	2	LCC	C2'-C3'	-3.20	1.46	1.53
1	AAA	2	LCC	C4'-C3'	-3.12	1.50	1.53
1	AAA	1	LCC	C2-N3	-3.11	1.30	1.36
1	AAA	3	LCC	C5M-C5	-3.09	1.43	1.50
1	AAA	2	LCC	C5M-C5	-3.06	1.43	1.50
1	BBB	15	G46	C5-C6	-3.06	1.33	1.44
1	BBB	2	LCC	O4'-C1'	-2.97	1.38	1.42
1	BBB	1	LCC	C6-N1	2.96	1.43	1.38
1	BBB	4	LCG	C4'-C3'	-2.87	1.50	1.53
1	BBB	1	LCC	C6-C5	2.80	1.39	1.34
1	BBB	3	LCC	O2'-C6'	2.80	1.48	1.43
1	AAA	2	LCC	C6-C5	2.77	1.39	1.34
1	BBB	3	LCC	C6-C5	2.77	1.39	1.34
1	AAA	15	G46	C5-N7	-2.69	1.33	1.39
1	BBB	4	LCG	C6'-C4'	-2.67	1.48	1.53
1	BBB	1	LCC	O4'-C1'	2.61	1.46	1.42
1	AAA	1	LCC	O4'-C4'	-2.56	1.42	1.45
1	BBB	1	LCC	C2-N1	-2.56	1.34	1.40
1	AAA	2	LCC	C6-N1	2.49	1.42	1.38
1	AAA	2	LCC	C2-N1	-2.48	1.34	1.40
1	AAA	15	G46	C5-C6	-2.44	1.35	1.44
1	AAA	3	LCC	C5-C4	-2.44	1.42	1.44
1	BBB	2	LCC	C6-C5	2.42	1.38	1.34
1	BBB	15	G46	C4-N9	-2.38	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	3	LCC	C6-N1	2.37	1.42	1.38
1	AAA	3	LCC	C6'-C4'	-2.32	1.48	1.53
1	BBB	2	LCC	C6'-C4'	2.26	1.57	1.53
1	BBB	3	LCC	C6'-C4'	-2.25	1.48	1.53
1	BBB	4	LCG	O2'-C6'	2.25	1.47	1.43
1	AAA	2	LCC	O3'-C3'	2.23	1.47	1.42
1	AAA	2	LCC	O2'-C6'	2.13	1.47	1.43
1	BBB	3	LCC	C2-N1	-2.12	1.35	1.40
1	BBB	15	G46	C6-N1	2.04	1.42	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	1	LCC	C5-C6-N1	-6.16	116.62	123.31
1	BBB	15	G46	O4'-C4'-C3'	-5.51	94.22	105.15
1	BBB	2	LCC	C5M-C5-C6	-5.06	116.00	122.85
1	BBB	2	LCC	C5-C6-N1	-4.95	117.93	123.31
1	BBB	3	LCC	C5-C6-N1	-4.88	118.02	123.31
1	BBB	1	LCC	O5'-C5'-C4'	-4.21	103.50	111.83
1	BBB	1	LCC	O4'-C4'-C5'	3.53	115.11	108.86
1	AAA	15	G46	O6-C6-N1	-3.51	113.52	120.11
1	AAA	1	LCC	O5'-C5'-C4'	-3.48	104.94	111.83
1	AAA	15	G46	C5-C4-N3	-3.33	123.09	128.39
1	AAA	1	LCC	O4'-C4'-C6'	3.33	113.02	105.97
1	BBB	2	LCC	O2'-C6'-C4'	-3.32	97.43	103.81
1	AAA	15	G46	C2-N1-C6	-3.26	119.19	125.11
1	AAA	1	LCC	C5M-C5-C6	-3.24	118.46	122.85
1	AAA	4	LCG	O2'-C6'-C4'	-3.24	97.59	103.81
1	AAA	15	G46	C4-C5-N7	-3.15	105.68	110.67
1	BBB	15	G46	C4-C5-N7	-3.12	105.72	110.67
1	AAA	2	LCC	C5M-C5-C6	-3.02	118.76	122.85
1	BBB	1	LCC	C5M-C5-C6	-2.97	118.83	122.85
1	AAA	1	LCC	C6-N1-C2	-2.89	117.09	120.95
1	AAA	1	LCC	C5M-C5-C4	2.85	125.20	120.51
1	AAA	3	LCC	C5-C4-N4	-2.85	117.38	121.39
1	AAA	15	G46	C2-N3-C4	2.83	117.18	112.30
1	AAA	15	G46	C8-N7-C5	2.76	109.18	104.26
1	AAA	1	LCC	C6'-O2'-C2'	-2.75	102.75	107.72
1	BBB	1	LCC	O4'-C4'-C3'	-2.74	98.50	102.32
1	AAA	4	LCG	C4-C5-N7	-2.71	106.38	110.67
1	BBB	3	LCC	C5-C4-N3	2.69	124.51	121.75
1	AAA	2	LCC	C5-C6-N1	-2.61	120.48	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	4	LCG	N1-C2-N3	-2.60	118.57	123.32
1	AAA	1	LCC	C5-C4-N4	-2.52	117.85	121.39
1	BBB	3	LCC	C4'-O4'-C1'	-2.49	103.20	107.77
1	BBB	1	LCC	O2-C2-N3	-2.44	118.48	122.33
1	AAA	2	LCC	O2'-C6'-C4'	-2.39	99.23	103.81
1	BBB	3	LCC	C6'-O2'-C2'	-2.37	103.45	107.72
1	AAA	4	LCG	C8-N7-C5	2.37	108.47	104.26
1	BBB	15	G46	C5'-C4'-C3'	2.30	123.48	115.21
1	AAA	4	LCG	C5-C4-N3	-2.26	124.79	128.39
1	AAA	1	LCC	O2'-C6'-C4'	-2.24	99.51	103.81
1	AAA	15	G46	N9-C8-N7	-2.23	109.27	113.40
1	BBB	3	LCC	C5M-C5-C6	-2.22	119.84	122.85
1	BBB	2	LCC	O2-C2-N3	-2.19	118.88	122.33
1	BBB	15	G46	O6-C6-N1	-2.19	116.00	120.11
1	AAA	4	LCG	C5-C4-N9	2.14	109.49	105.66
1	BBB	1	LCC	O4'-C4'-C6'	2.11	110.43	105.97
1	BBB	2	LCC	C5M-C5-C4	2.11	123.97	120.51
1	AAA	2	LCC	C5M-C5-C4	2.10	123.95	120.51
1	AAA	4	LCG	N9-C8-N7	-2.07	109.57	113.40
1	AAA	15	G46	C6-C5-N7	2.04	134.00	130.29
1	BBB	1	LCC	O2'-C6'-C4'	-2.03	99.91	103.81
1	AAA	15	G46	C5-C6-N1	2.00	118.35	113.25

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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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
3	DGP	BBB	102	-	25,25,25	1.43	4 (16%)	37,38,38	1.95	10 (27%)
3	DGP	BBB	101	-	25,25,25	1.53	5 (20%)	37,38,38	1.92	10 (27%)

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	DGP	BBB	102	-	-	2/10/22/22	0/3/3/3
3	DGP	BBB	101	-	-	3/10/22/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	101	DGP	C5-N7	-3.54	1.32	1.39
3	BBB	102	DGP	C5-C6	-3.25	1.32	1.44
3	BBB	101	DGP	C5-C6	-3.18	1.32	1.44
3	BBB	102	DGP	O4'-C1'	2.78	1.48	1.42
3	BBB	101	DGP	C8-N9	-2.55	1.31	1.37
3	BBB	101	DGP	C4-N9	-2.51	1.31	1.38
3	BBB	102	DGP	C8-N9	-2.43	1.32	1.37
3	BBB	101	DGP	C6-N1	2.27	1.43	1.38
3	BBB	102	DGP	C5-N7	-2.22	1.34	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	102	DGP	C2-N1-C6	-4.77	116.46	125.11
3	BBB	101	DGP	C2-N3-C4	4.71	120.41	112.30
3	BBB	101	DGP	C2-N1-C6	-4.64	116.70	125.11
3	BBB	102	DGP	C2-N3-C4	4.33	119.75	112.30
3	BBB	101	DGP	C5-C4-N3	-4.16	121.77	128.39
3	BBB	102	DGP	C5-C4-N3	-3.86	122.25	128.39
3	BBB	102	DGP	C5-C6-N1	3.25	121.53	113.25
3	BBB	101	DGP	C5-C6-N1	3.06	121.05	113.25
3	BBB	102	DGP	N9-C8-N7	-2.98	107.88	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	102	DGP	O6-C6-N1	-2.45	115.50	120.11
3	BBB	101	DGP	C2'-C3'-C4'	2.44	107.74	102.80
3	BBB	101	DGP	O5'-P-OP1	-2.44	99.85	106.44
3	BBB	102	DGP	OP3-P-OP2	2.43	116.92	107.80
3	BBB	101	DGP	N9-C4-N3	2.43	130.81	125.95
3	BBB	102	DGP	C4'-O4'-C1'	-2.41	103.79	109.51
3	BBB	101	DGP	N9-C8-N7	-2.40	108.95	113.40
3	BBB	102	DGP	N9-C4-N3	2.38	130.72	125.95
3	BBB	102	DGP	C8-N7-C5	2.32	108.39	104.26
3	BBB	101	DGP	OP3-P-OP2	2.27	116.31	107.80
3	BBB	101	DGP	C8-N7-C5	2.15	108.09	104.26

There are no chirality outliers.

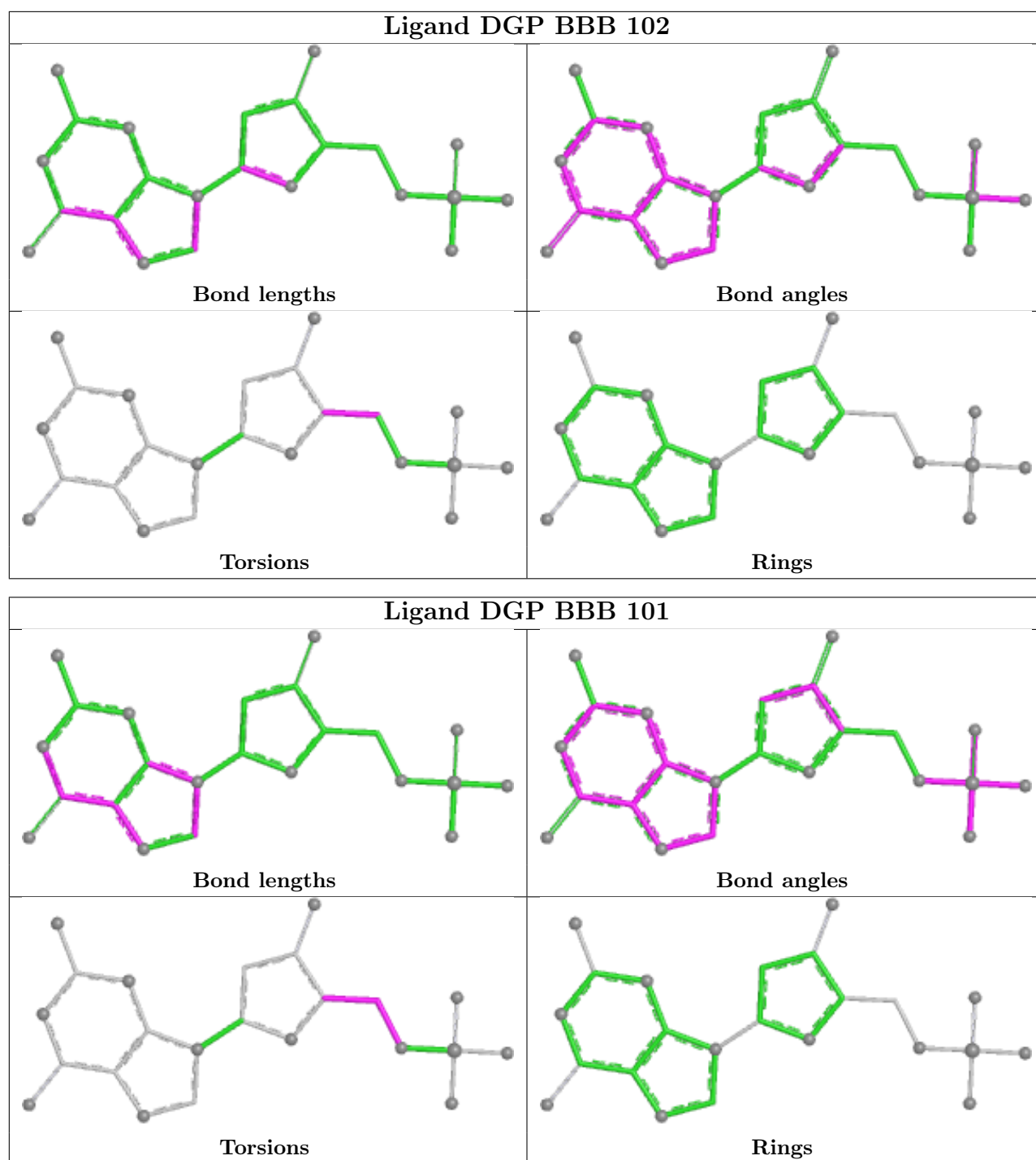
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	101	DGP	O4'-C4'-C5'-O5'
3	BBB	102	DGP	O4'-C4'-C5'-O5'
3	BBB	102	DGP	C3'-C4'-C5'-O5'
3	BBB	101	DGP	C3'-C4'-C5'-O5'
3	BBB	101	DGP	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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	10/15 (66%)	-0.33	0 100 100	9, 13, 15, 16	0
1	BBB	10/15 (66%)	-0.33	0 100 100	10, 13, 14, 16	0
All	All	20/30 (66%)	-0.33	0 100 100	9, 13, 16, 16	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
1	LCC	BBB	1	19/23	0.87	0.13	17,23,29,33	0
1	LCC	AAA	1	19/23	0.92	0.10	14,17,20,23	0
1	G46	AAA	15	23/24	0.94	0.10	14,20,27,30	0
1	LCC	BBB	2	22/23	0.96	0.07	14,15,19,23	0
1	G46	BBB	15	23/24	0.96	0.07	10,12,20,21	0
1	LCC	AAA	2	22/23	0.97	0.06	9,11,15,17	0
1	LCG	AAA	4	24/25	0.98	0.05	8,9,10,10	0
1	LCG	BBB	4	24/25	0.98	0.05	9,10,11,12	0
1	LCC	AAA	3	22/23	0.98	0.05	8,9,11,13	0
1	LCC	BBB	3	22/23	0.98	0.05	10,11,14,16	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

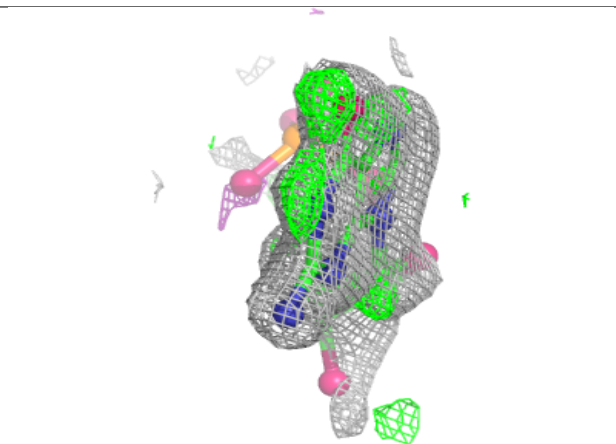
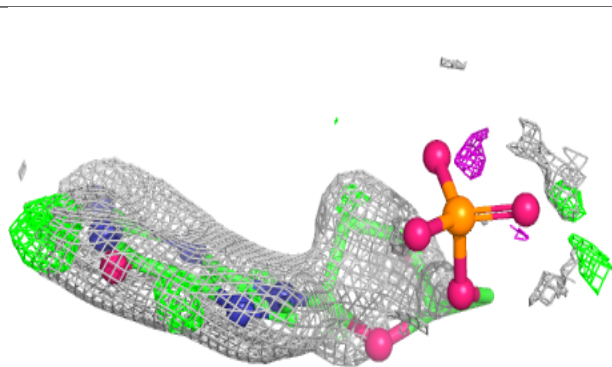
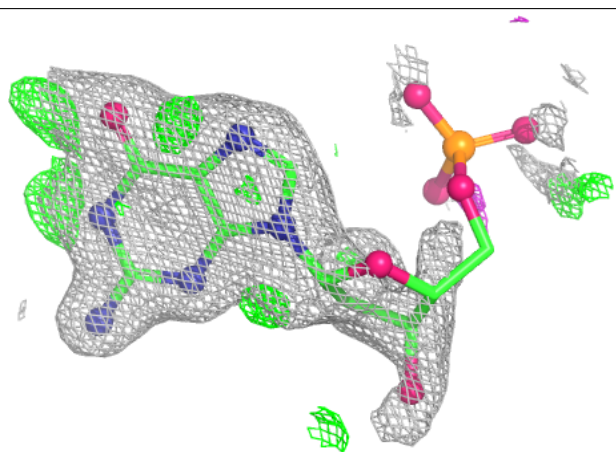
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DGP	BBB	101	23/23	0.83	0.19	19,25,120,128	0
3	DGP	BBB	102	23/23	0.87	0.15	16,24,103,104	0
2	MG	BBB	104	1/1	0.89	0.11	42,42,42,42	0
2	MG	BBB	105	1/1	0.89	0.09	24,24,24,24	1
2	MG	AAA	102	1/1	0.95	0.07	27,27,27,27	0
2	MG	AAA	101	1/1	0.98	0.09	12,12,12,12	0
2	MG	BBB	103	1/1	0.99	0.04	10,10,10,10	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.

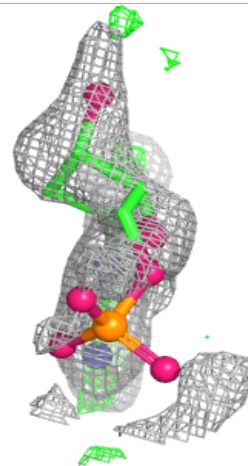
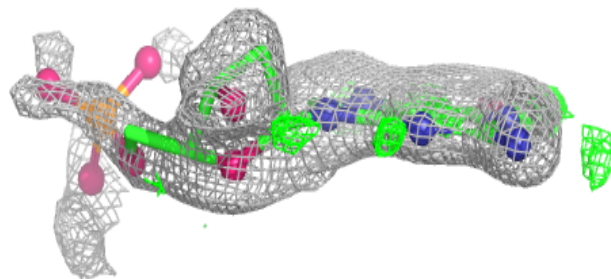
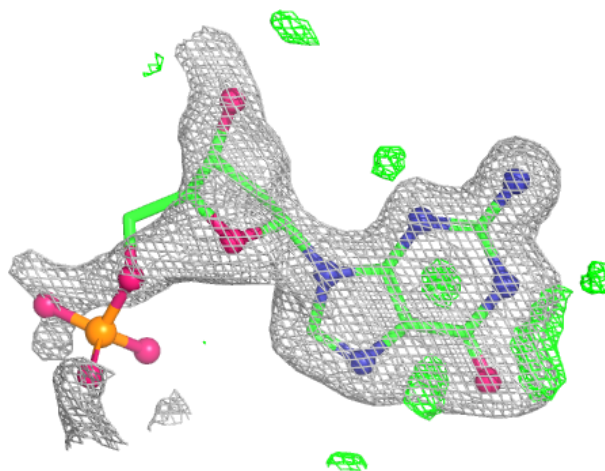
Electron density around DGP BBB 101:

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 DGP BBB 102:

$2mF_o-DF_c$ (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.