



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:50 PM EDT

PDB ID : 3R1D / pdb_00003r1d
Title : Crystal structure of GC(8BrG)GCGGCGGC duplex
Authors : Kiliszek, A.; Kierzek, R.; Krzyzosiak, W.J.; Rypniewski, W.
Deposited on : 2011-03-10
Resolution : 1.45 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 1.45 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1871 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.

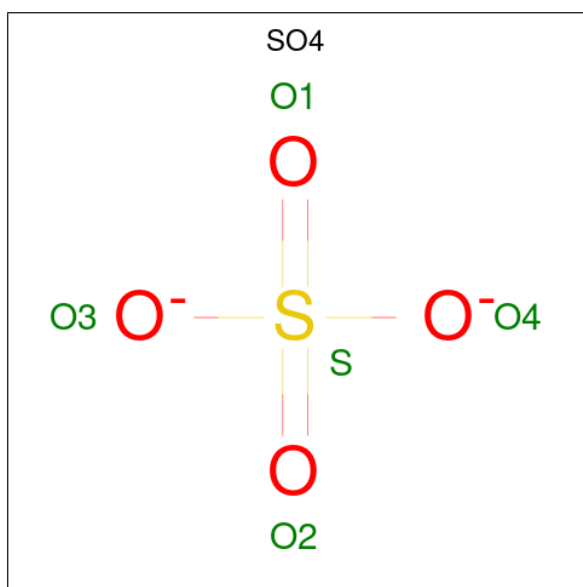
- Molecule 1 is a RNA chain called RNA (5'-R(*GP*CP*(GRB)P*GP*CP*GP*GP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	11	Total	Br	C	N	O	P	0	4	0
			326	2	145	65	101	13			
1	B	11	Total	Br	C	N	O	P	0	2	0
			279	1	125	55	87	11			
1	C	11	Total	Br	C	N	O	P	0	6	0
			355	2	157	70	111	15			
1	D	11	Total	Br	C	N	O	P	0	2	0
			285	1	126	57	89	12			
1	E	11	Total	Br	C	N	O	P	0	6	0
			372	2	165	75	115	15			

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Br	0	0
			1	1		
2	B	1	Total	Br	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	1
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	1
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	1
			5	4	1		
3	E	1	Total	O	S	0	1
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	1
			47	47		
4	B	47	Total	O	0	2
			49	49		
4	C	40	Total	O	0	1
			40	40		
4	D	45	Total	O	0	4
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	27	Total	O	0	1
			27	27		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.56Å 28.61Å 61.83Å 90.00° 117.98° 90.00°	Depositor
Resolution (Å)	19.97 – 1.45	Depositor
% Data completeness (in resolution range)	98.9 (19.97-1.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.232 , 0.270	Depositor
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.042	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1871	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

8 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	GRB	A	3[A]	1	23,26,27	0.58	1 (4%)	32,39,42	1.09	1 (3%)
1	GRB	A	3[B]	1	23,26,27	0.55	0	32,39,42	0.77	1 (3%)
1	GRB	B	3	1	23,26,27	0.82	1 (4%)	32,39,42	1.17	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GRB	C	3[A]	1	23,26,27	0.77	1 (4%)	32,39,42	1.27	2 (6%)
1	GRB	E	3[A]	1	23,26,27	0.62	1 (4%)	32,39,42	0.75	1 (3%)
1	GRB	E	3[B]	1	23,26,27	0.61	1 (4%)	32,39,42	1.00	1 (3%)
1	GRB	C	3[B]	1	23,26,27	0.54	0	32,39,42	0.76	1 (3%)
1	GRB	D	3	1	23,26,27	0.64	0	32,39,42	0.85	1 (3%)

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	GRB	A	3[A]	1	-	3/7/25/26	0/3/3/3
1	GRB	A	3[B]	1	-	3/7/25/26	0/3/3/3
1	GRB	B	3	1	-	3/7/25/26	0/3/3/3
1	GRB	C	3[A]	1	-	3/7/25/26	0/3/3/3
1	GRB	E	3[A]	1	-	3/7/25/26	0/3/3/3
1	GRB	E	3[B]	1	-	3/7/25/26	0/3/3/3
1	GRB	C	3[B]	1	-	3/7/25/26	0/3/3/3
1	GRB	D	3	1	-	3/7/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GRB	BR-C8	3.36	1.92	1.86
1	C	3[A]	GRB	BR-C8	3.26	1.92	1.86
1	E	3[A]	GRB	BR-C8	2.33	1.90	1.86
1	E	3[B]	GRB	BR-C8	2.20	1.90	1.86
1	A	3[A]	GRB	BR-C8	2.06	1.90	1.86

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3[A]	GRB	C2'-C1'-N9	-5.19	108.95	115.90
1	E	3[B]	GRB	C2'-C1'-N9	-4.70	109.60	115.90
1	A	3[A]	GRB	C2'-C1'-N9	-4.50	109.87	115.90
1	B	3	GRB	C2'-C1'-N9	-4.21	110.25	115.90
1	B	3	GRB	N9-C8-N7	-3.43	112.37	115.04
1	C	3[B]	GRB	C2'-C1'-N9	-3.26	111.53	115.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3[B]	GRB	C2'-C1'-N9	-3.20	111.61	115.90
1	C	3[A]	GRB	N9-C8-N7	-3.16	112.59	115.04
1	E	3[A]	GRB	C2'-C1'-N9	-2.60	112.41	115.90
1	D	3	GRB	BR-C8-N9	2.28	124.24	121.97

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	3[A]	GRB	O4'-C1'-N9-C4
1	A	3[A]	GRB	O4'-C1'-N9-C8
1	A	3[B]	GRB	O4'-C1'-N9-C4
1	A	3[B]	GRB	O4'-C1'-N9-C8
1	B	3	GRB	O4'-C1'-N9-C4
1	B	3	GRB	O4'-C1'-N9-C8
1	C	3[A]	GRB	O4'-C1'-N9-C4
1	C	3[A]	GRB	O4'-C1'-N9-C8
1	C	3[B]	GRB	O4'-C1'-N9-C4
1	C	3[B]	GRB	O4'-C1'-N9-C8
1	D	3	GRB	O4'-C1'-N9-C4
1	D	3	GRB	O4'-C1'-N9-C8
1	E	3[A]	GRB	O4'-C1'-N9-C4
1	E	3[A]	GRB	O4'-C1'-N9-C8
1	E	3[B]	GRB	O4'-C1'-N9-C4
1	E	3[B]	GRB	O4'-C1'-N9-C8
1	A	3[A]	GRB	C2'-C1'-N9-C4
1	C	3[A]	GRB	C2'-C1'-N9-C4
1	E	3[B]	GRB	C2'-C1'-N9-C4
1	C	3[B]	GRB	C2'-C1'-N9-C4
1	E	3[A]	GRB	C2'-C1'-N9-C4
1	B	3	GRB	C2'-C1'-N9-C4
1	A	3[B]	GRB	C2'-C1'-N9-C4
1	D	3	GRB	C2'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	SO4	C	13[B]	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	12	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	13	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	A	14[A]	-	4,4,4	0.21	0	6,6,6	0.06	0
3	SO4	E	12[B]	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	E	13[A]	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	12	-	4,4,4	0.25	0	6,6,6	0.26	0
3	SO4	B	13	-	4,4,4	0.21	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.