



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:20 am BST

PDB ID : 1N7A
Title : RIP-Radiation-damage Induced Phasing
Authors : Ravelli, R.B.G.; Leiros, H.-K.S.; Pan, B.; Caffrey, M.; McSweeney, S.
Deposited on : 2002-11-13
Resolution : 1.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

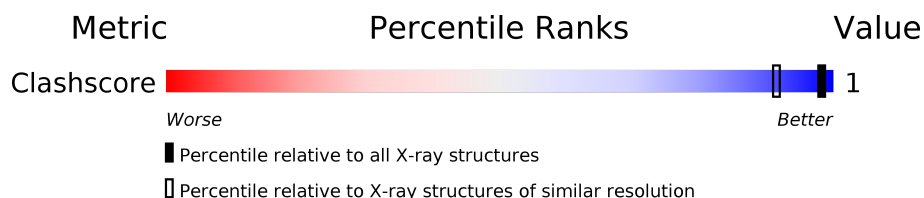
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
Clashscore	141614	1286 (1.22-1.18)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	6	 100%
1	B	6	 83% 17%
1	C	6	 100%
1	D	6	 100%
1	E	6	 100%
1	F	6	 100%
1	G	6	 100%
1	H	6	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1236 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.

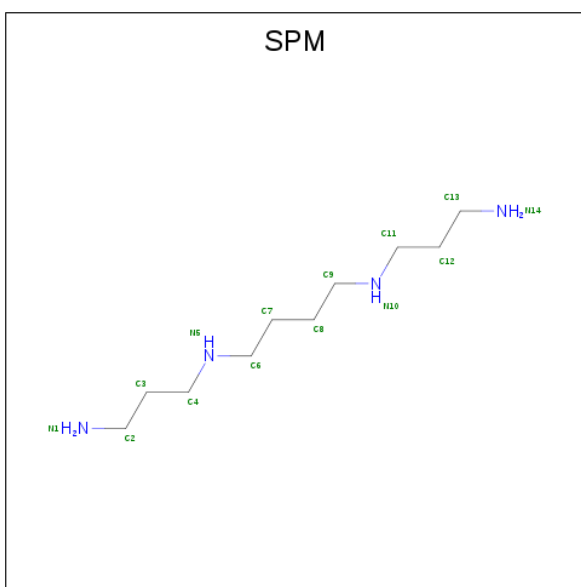
- Molecule 1 is DNA/RNA hybrid called RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	B	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	C	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	D	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	E	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	F	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	G	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			
1	H	6	Total	Br	C	N	O	P	0	0	0
			128	1	58	24	40	5			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	K	0	0
			3	3		
2	A	5	Total	K	0	0
			5	5		
2	E	1	Total	K	0	0
			1	1		

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			14	10	4		
3	H	1	Total	C	N	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	24	Total	O	0	0
			24	24		
4	C	25	Total	O	0	0
			25	25		
4	D	16	Total	O	0	0
			16	16		
4	E	19	Total	O	0	0
			19	19		
4	F	23	Total	O	0	0
			23	23		
4	G	30	Total	O	0	0
			30	30		
4	H	24	Total	O	0	0
			24	24		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.


Note EDS was not executed.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain B:  83% 17%



- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA/DNA (5'-R(*U)-D(P*(BGM))-R(P*AP*GP*GP*U)-3')

Chain H:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	31.23 Å 51.10 Å 70.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.20	Depositor
% Data completeness (in resolution range)	99.7 (20.00-1.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.124 , 0.156	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1236	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

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: K, SPM, BGM

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	1.03	0/117	1.36	0/181
1	B	1.04	0/117	1.40	0/181
1	C	0.87	0/117	1.28	0/181
1	D	0.88	0/117	1.21	0/181
1	E	0.96	0/117	1.35	0/181
1	F	0.85	0/117	1.38	0/181
1	G	0.95	0/117	1.38	0/181
1	H	0.84	0/117	1.37	0/181
All	All	0.93	0/936	1.34	0/1448

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	128	0	65	0	0
1	B	128	0	65	1	0
1	C	128	0	65	0	0
1	D	128	0	65	0	0
1	E	128	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	128	0	65	0	0
1	G	128	0	65	0	0
1	H	128	0	65	0	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
2	E	1	0	0	0	0
3	B	14	0	26	1	0
3	H	8	0	13	0	0
4	A	20	0	0	0	0
4	B	24	0	0	0	0
4	C	25	0	0	0	0
4	D	16	0	0	0	0
4	E	19	0	0	0	0
4	F	23	0	0	0	0
4	G	30	0	0	0	0
4	H	24	0	0	0	0
All	All	1236	0	559	1	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 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:B:2:BGM:OP1	3:B:502:SPM:H62	1.79	0.82

There are no symmetry-related clashes.

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 ⓘ

There are no RNA molecules in this entry.

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

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	BGM	E	2	1,2	19,25,26	1.34	3 (15%)	20,37,40	2.54	5 (25%)
1	BGM	H	2	1,2	19,25,26	1.42	3 (15%)	20,37,40	2.56	6 (30%)
1	BGM	F	2	1,2	19,25,26	1.29	2 (10%)	20,37,40	2.42	6 (30%)
1	BGM	A	2	1,2	19,25,26	1.25	2 (10%)	20,37,40	2.28	6 (30%)
1	BGM	D	2	1,2	19,25,26	1.37	2 (10%)	20,37,40	2.30	5 (25%)
1	BGM	G	2	1,2	19,25,26	1.20	2 (10%)	20,37,40	2.60	5 (25%)
1	BGM	B	2	1,2	19,25,26	1.47	3 (15%)	20,37,40	2.46	5 (25%)
1	BGM	C	2	1,2	19,25,26	1.23	2 (10%)	20,37,40	2.62	5 (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	BGM	E	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	H	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	F	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	A	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	D	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	G	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	B	2	1,2	-	2/3/21/22	0/3/3/3
1	BGM	C	2	1,2	-	2/3/21/22	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	BGM	C6-N1	4.51	1.40	1.33
1	D	2	BGM	C6-N1	4.51	1.40	1.33
1	H	2	BGM	C6-N1	4.43	1.40	1.33
1	F	2	BGM	C6-N1	4.22	1.40	1.33
1	E	2	BGM	C6-N1	3.93	1.39	1.33
1	C	2	BGM	C6-N1	3.91	1.39	1.33
1	A	2	BGM	C6-N1	3.45	1.39	1.33
1	G	2	BGM	C6-N1	3.19	1.38	1.33
1	E	2	BGM	C8-N7	-2.88	1.30	1.34
1	A	2	BGM	C8-N7	-2.70	1.30	1.34
1	B	2	BGM	C8-N7	-2.70	1.30	1.34
1	F	2	BGM	C8-N7	-2.26	1.31	1.34
1	G	2	BGM	C8-N7	-2.24	1.31	1.34
1	H	2	BGM	C8-N7	-2.24	1.31	1.34
1	D	2	BGM	C8-N7	-2.14	1.31	1.34
1	B	2	BGM	C2-N1	2.13	1.39	1.35
1	H	2	BGM	C8-N9	2.11	1.39	1.34
1	C	2	BGM	C8-N7	-2.03	1.31	1.34
1	E	2	BGM	C2-N1	2.00	1.39	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	BGM	C5-C6-N1	-8.48	111.84	123.43
1	C	2	BGM	C5-C6-N1	-8.28	112.11	123.43
1	H	2	BGM	C5-C6-N1	-7.98	112.52	123.43
1	F	2	BGM	C5-C6-N1	-7.92	112.59	123.43
1	B	2	BGM	C5-C6-N1	-7.69	112.91	123.43
1	A	2	BGM	C5-C6-N1	-7.44	113.26	123.43
1	G	2	BGM	C5-C6-N1	-7.33	113.41	123.43
1	D	2	BGM	C5-C6-N1	-6.71	114.26	123.43
1	C	2	BGM	C6-N1-C2	5.84	125.21	115.93
1	G	2	BGM	C6-N1-C2	5.62	124.86	115.93
1	E	2	BGM	C6-N1-C2	5.46	124.60	115.93
1	B	2	BGM	C6-N1-C2	5.25	124.26	115.93
1	H	2	BGM	C6-N1-C2	5.21	124.20	115.93
1	F	2	BGM	C6-N1-C2	5.07	123.99	115.93
1	D	2	BGM	C6-N1-C2	4.73	123.45	115.93
1	A	2	BGM	C6-N1-C2	4.64	123.31	115.93
1	G	2	BGM	C6-C5-C4	-3.82	117.15	120.80
1	D	2	BGM	C6-C5-C4	-3.60	117.36	120.80
1	B	2	BGM	N3-C2-N1	-3.50	122.55	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2	BGM	N3-C2-N1	-3.44	122.64	127.22
1	G	2	BGM	C4-C5-N7	3.37	112.88	109.47
1	D	2	BGM	N3-C2-N1	-3.31	122.81	127.22
1	C	2	BGM	N3-C2-N1	-3.21	122.94	127.22
1	H	2	BGM	C4-C5-N7	3.12	112.63	109.47
1	H	2	BGM	N3-C2-N1	-3.03	123.18	127.22
1	E	2	BGM	N3-C2-N1	-2.81	123.47	127.22
1	C	2	BGM	C2-N3-C4	-2.80	112.16	115.36
1	H	2	BGM	C6-C5-C4	-2.79	118.13	120.80
1	F	2	BGM	N3-C2-N1	-2.72	123.60	127.22
1	H	2	BGM	C2-N3-C4	-2.69	112.28	115.36
1	F	2	BGM	C6-C5-C4	-2.64	118.28	120.80
1	B	2	BGM	C2-N3-C4	-2.54	112.45	115.36
1	A	2	BGM	C2-N3-C4	-2.46	112.55	115.36
1	A	2	BGM	C6-C5-C4	-2.43	118.48	120.80
1	F	2	BGM	C4-C5-N7	2.42	111.92	109.47
1	E	2	BGM	C2-N3-C4	-2.38	112.64	115.36
1	B	2	BGM	C6-C5-C4	-2.20	118.69	120.80
1	F	2	BGM	C2-N3-C4	-2.17	112.88	115.36
1	A	2	BGM	N3-C2-N1	-2.15	124.36	127.22
1	E	2	BGM	C4-C5-N7	2.10	111.60	109.47
1	C	2	BGM	C6-C5-C4	-2.07	118.82	120.80
1	D	2	BGM	C2-N3-C4	-2.03	113.04	115.36
1	A	2	BGM	C4-C5-N7	2.00	111.50	109.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	2	BGM	O4'-C4'-C5'-O5'
1	C	2	BGM	O4'-C4'-C5'-O5'
1	H	2	BGM	C3'-C4'-C5'-O5'
1	B	2	BGM	O4'-C4'-C5'-O5'
1	E	2	BGM	O4'-C4'-C5'-O5'
1	C	2	BGM	C3'-C4'-C5'-O5'
1	F	2	BGM	O4'-C4'-C5'-O5'
1	D	2	BGM	O4'-C4'-C5'-O5'
1	G	2	BGM	O4'-C4'-C5'-O5'
1	B	2	BGM	C3'-C4'-C5'-O5'
1	A	2	BGM	O4'-C4'-C5'-O5'
1	E	2	BGM	C3'-C4'-C5'-O5'
1	D	2	BGM	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	G	2	BGM	C3'-C4'-C5'-O5'
1	F	2	BGM	C3'-C4'-C5'-O5'
1	A	2	BGM	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	2	BGM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 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	SPM	H	501	-	7,7,13	0.43	0	5,6,12	0.43	0
3	SPM	B	502	-	13,13,13	0.30	0	12,12,12	0.96	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
3	SPM	H	501	-	-	0/5/5/11	-
3	SPM	B	502	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	SPM	N5-C6-C7-C8
3	B	502	SPM	N10-C11-C12-C13
3	B	502	SPM	C7-C8-C9-N10
3	B	502	SPM	C8-C9-N10-C11

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	SPM	1	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.