wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 06:23 pm BST

PDB ID	:	2JJA / pdb_00002jja
Title	:	Crystal structure of GNA with synthetic copper base pair
Authors	:	Schlegel, M.K.; Essen, L.-O.; Meggers, E.
Deposited on	:	2008-03-28
Resolution	:	1.30 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 (i) 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 (1)) were used in the production of this report:

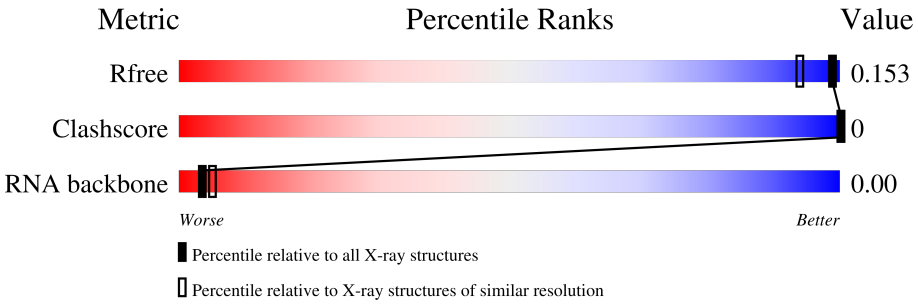
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
RNA backbone	3983	1020 (2.10-0.62)

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 <=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	8	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	ZHP	A	3	X	-	-	-
1	ZHP	A	6	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 234 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 GNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	8	136	64	25	40	7	0	0	0

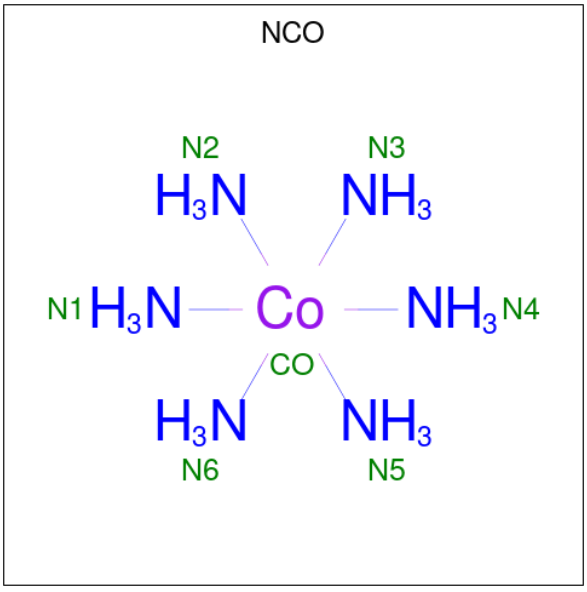
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0

- Molecule 4 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Co N 7 1 6	0	0
4	A	1	Total Co N 7 1 6	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

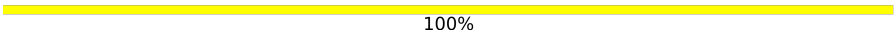
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	80	Total O 80 80	0	0

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: GNA

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	18.16Å 48.59Å 59.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.30 10.00 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-1.30) 98.6 (10.00-1.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.124 , 0.148 0.133 , 0.153	Depositor DCC
R_{free} test set	479 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	234	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 21.03 % 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 7.6480e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, ZAD, NCO, ZHP, ZTH, MG, ZGU, CU, ZCY

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	ZHP	C2
1	A	6	ZHP	C2

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	A	136	0	76	0	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	0	0	0
5	A	1	0	0	0	0
6	A	80	0	0	0	0
All	All	234	0	76	0	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 0.

There are no clashes within the asymmetric unit.

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 (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/8	-	-

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 (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	ZAD	A	4	1	16,19,20	0.83	2 (12%)	21,26,29	1.95	6 (28%)
1	ZCY	A	7	1	13,16,17	1.13	1 (7%)	14,21,24	1.69	2 (14%)
1	ZCY	A	1	1	13,13,17	1.64	3 (23%)	14,17,24	1.36	2 (14%)
1	ZTH	A	5	1	14,17,18	1.50	4 (28%)	17,23,26	2.35	8 (47%)
1	ZGU	A	2	1	17,20,21	1.10	1 (5%)	22,28,31	1.45	5 (22%)
1	ZGU	A	8	1	17,20,21	1.24	2 (11%)	22,28,31	1.55	5 (22%)
1	ZHP	A	6	2,1	14,17,18	2.70	2 (14%)	15,23,26	3.46	9 (60%)
1	ZHP	A	3	2,1	14,17,18	3.22	2 (14%)	15,23,26	3.51	8 (53%)

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	ZAD	A	4	1	-	0/7/9/10	0/2/2/2
1	ZCY	A	7	1	-	0/7/9/10	0/1/1/1
1	ZCY	A	1	1	-	0/6/6/10	0/1/1/1
1	ZHP	A	6	2,1	1/1/2/2	0/7/9/10	0/1/1/1
1	ZGU	A	2	1	-	0/7/9/10	0/2/2/2
1	ZTH	A	5	1	-	1/7/9/10	0/1/1/1
1	ZGU	A	8	1	-	0/7/9/10	0/2/2/2
1	ZHP	A	3	2,1	1/1/2/2	0/7/9/10	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	ZHP	C3-C2	11.44	1.47	1.37
1	A	6	ZHP	C3-C2	9.28	1.45	1.37
1	A	1	ZCY	C2-N1	-4.69	1.34	1.40
1	A	5	ZTH	C4-C5	-2.99	1.39	1.44
1	A	8	ZGU	C4-N9	-2.68	1.33	1.37

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	ZHP	C2-C3-C4	-8.70	117.51	122.52
1	A	6	ZHP	O3-C3-C2	7.24	125.34	118.36
1	A	6	ZHP	C2-C3-C4	-5.59	119.30	122.52
1	A	3	ZHP	C1G-N1-C2	-5.54	117.84	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ZHP	C1G-N1-C2	-4.98	118.21	121.46

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	ZHP	C2
1	A	6	ZHP	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	5	ZTH	C1G-C2G-C3G-O3G

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, 4 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	$\#\|Z\| > 2$
4	NCO	A	1004	-	6,6,6	0.66	0	-		
4	NCO	A	1005	-	6,6,6	0.47	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.

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

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, 95^{th} 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	0/8	-	-	-	-

There are no RSRZ outliers to report.

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

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, 95^{th} 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	ZAD	A	4	18/19	0.97	0.07	16,18,23,24	0
1	ZHP	A	3	17/18	0.97	0.07	15,16,27,28	0
1	ZTH	A	5	17/18	0.98	0.05	16,18,25,26	0
1	ZCY	A	1	13/17	0.98	0.05	14,15,16,16	0
1	ZHP	A	6	17/18	0.98	0.06	15,17,28,30	0
1	ZGU	A	8	19/20	0.99	0.05	13,15,16,16	0
1	ZGU	A	2	19/20	0.99	0.04	12,14,17,20	0
1	ZCY	A	7	16/17	0.99	0.04	13,14,22,22	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
5	NA	A	1006	1/1	0.72	0.10	78,78,78,78	0
4	NCO	A	1005	7/7	0.98	0.09	26,26,27,28	7
4	NCO	A	1004	7/7	0.99	0.09	18,20,22,22	7
3	MG	A	1002	1/1	0.99	0.04	22,22,22,22	0
3	MG	A	1003	1/1	0.99	0.03	24,24,24,24	1
2	CU	A	1001	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.