



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2022 – 12:22 PM EDT

PDB ID : 5V1L
Title : Structure of S-GNA dodecamer
Authors : Pallan, P.S.; Egli, M.
Deposited on : 2017-03-02
Resolution : 1.20 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 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) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

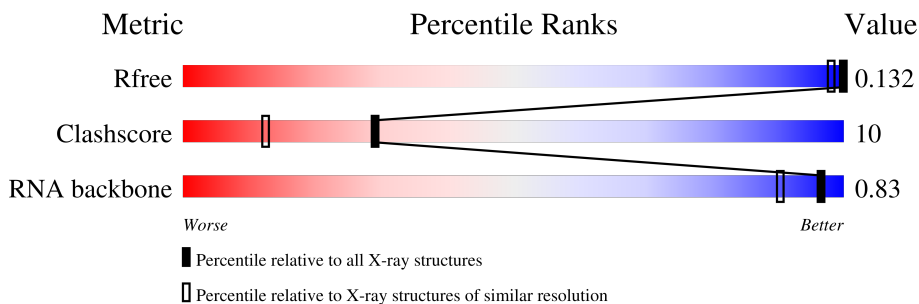
1 Overall quality at a glance

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))
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
RNA backbone	3102	1000 (2.34-0.62)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	12	42% 50% 8%
1	B	12	33% 58% 8%
1	C	12	42% 58%
1	D	12	33% 67%

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
3	SPM	B	303	-	X	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 1419 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(*CP*GP*CP*GP*AP*AP*UP*(ZTH)P*AP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	12	Total 284	C 126	N 50	O 94	P 14	0	3	0
1	B	12	Total 252	C 114	N 48	O 79	P 11	0	0	0
1	C	12	Total 252	C 114	N 48	O 79	P 11	0	0	0
1	D	12	Total 275	C 124	N 50	O 88	P 13	0	2	0

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Sr 1	0	0
2	B	2	Total 2	Sr 2	0	0
2	C	4	Total 4	Sr 4	0	0
2	D	1	Total 1	Sr 1	0	0

- 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		

- Molecule 4 is water.

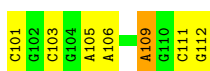
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	65	Total	O	0	0
			65	65		
4	C	95	Total	O	0	0
			95	95		
4	D	94	Total	O	0	0
			94	94		

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. 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.

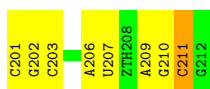
- Molecule 1: RNA (5'-R(*CP*GP*CP*GP*AP*AP*UP*(ZTH)P*AP*GP*CP*G)-3')

Chain A: 



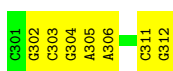
- Molecule 1: RNA (5'-R(*CP*GP*CP*GP*AP*AP*UP*(ZTH)P*AP*GP*CP*G)-3')

Chain B: 

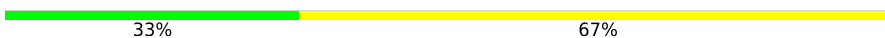


- Molecule 1: RNA (5'-R(*CP*GP*CP*GP*AP*AP*UP*(ZTH)P*AP*GP*CP*G)-3')

Chain C: 



- Molecule 1: RNA (5'-R(*CP*GP*CP*GP*AP*AP*UP*(ZTH)P*AP*GP*CP*G)-3')

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	34.95Å 46.24Å 82.93Å 90.00° 100.09° 90.00°	Depositor
Resolution (Å)	27.60 – 1.20 27.61 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.60-1.20) 99.8 (27.61-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.20Å)	Xtrriage
Refinement program	SHELXL	Depositor
R, R_{free}	(Not available) , 0.153 0.129 , 0.132	Depositor DCC
R_{free} test set	2039 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	1419	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.09 % 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 1.1722e-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: SPM, SR, ZTH

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	1.42	2/308 (0.6%)	1.94	9/474 (1.9%)
1	B	1.48	3/262 (1.1%)	2.22	18/405 (4.4%)
1	C	1.52	1/262 (0.4%)	2.19	16/405 (4.0%)
1	D	1.48	0/287	2.12	14/444 (3.2%)
All	All	1.47	6/1119 (0.5%)	2.11	57/1728 (3.3%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	C	C2'-O2'	9.52	1.54	1.41
1	B	207	U	C2'-O2'	-6.25	1.33	1.41
1	B	201	C	C2'-O2'	6.03	1.49	1.41
1	B	211	C	C2'-O2'	6.01	1.49	1.41
1	A	105	A	C2'-O2'	5.21	1.48	1.41

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	A	N1-C6-N6	9.47	124.28	118.60
1	C	305	A	N7-C8-N9	-9.27	109.17	113.80
1	C	304	G	C5-N7-C8	8.15	108.37	104.30
1	C	303	C	N1-C2-O2	-8.09	114.05	118.90
1	D	411	C	N3-C4-C5	-8.06	118.67	121.90

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	284	0	137	2	0
1	B	252	0	132	1	0
1	C	252	0	131	0	0
1	D	275	0	139	3	0
2	A	1	0	0	0	0
2	B	2	0	0	1	0
2	C	4	0	0	0	0
2	D	1	0	0	0	0
3	B	14	0	18	12	0
4	A	80	0	0	1	0
4	B	65	0	0	1	0
4	C	95	0	0	0	0
4	D	94	0	0	1	0
All	All	1419	0	557	16	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 10.

The worst 5 of 16 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)
3:B:303:SPM:H62	3:B:303:SPM:C2	1.68	1.18
3:B:303:SPM:H62	3:B:303:SPM:N1	1.83	0.94
3:B:303:SPM:H82	3:B:303:SPM:H122	1.56	0.87
3:B:303:SPM:C2	3:B:303:SPM:C6	2.55	0.83
2:B:301:SR:SR	2:B:302:SR:SR	1.44	0.72

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	8/12 (66%)	0	0
1	B	9/12 (75%)	0	0
1	C	9/12 (75%)	0	0
1	D	9/12 (75%)	0	0
All	All	35/48 (72%)	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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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	B	303	-	13,13,13	1.80	2 (15%)	12,12,12	3.89	7 (58%)

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	B	303	-	-	6/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	SPM	C2-N1	-5.19	1.04	1.46
3	B	303	SPM	C13-N14	-3.14	1.21	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	SPM	C8-C9-N10	6.88	130.70	112.14
3	B	303	SPM	C12-C13-N14	6.78	161.35	112.78
3	B	303	SPM	C3-C2-N1	6.60	160.05	112.78
3	B	303	SPM	C12-C11-N10	4.73	124.90	112.14
3	B	303	SPM	C7-C6-N5	2.82	119.74	112.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	SPM	C3-C4-N5-C6
3	B	303	SPM	C12-C11-N10-C9
3	B	303	SPM	C8-C9-N10-C11
3	B	303	SPM	N1-C2-C3-C4
3	B	303	SPM	N10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	SPM	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.