wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 02:20 PM GMT

PDB ID	:	1D99
Title	:	STRUCTURAL FEATURES AND HYDRATION OF A DODECAMER DUPLEX CONTAINING TWO C.A MISPAIRS
Authors	:	Hunter, W.N.; Brown, T.; Kennard, O.
Deposited on	:	1992-10-17
Resolution	:	2.50 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Clashscore		22

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
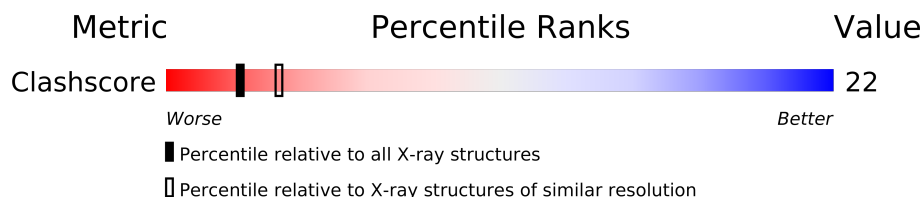
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	12	
1	B	12	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 562 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called DNA (5'-D(*CP*GP*CP*AP*AP*AP*TP*TP*CP*GP* CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	12	Total	C	N	O	P	0	0	0
			242	116	46	69	11			
1	B	12	Total	C	N	O	P	0	0	0
			242	116	46	69	11			

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	44	Total	O	0	0
			44	44		

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 errors 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.
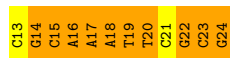
Note EDS was not executed.

• Molecule 1: DNA (5'-D(*CP*GP*CP*AP*AP*AP*TP*TP*CP*GP*CP*G)-3')

Chain A:
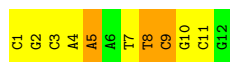
• Molecule 1: DNA (5'-D(*CP*GP*CP*AP*AP*AP*TP*TP*CP*GP*CP*G)-3')

Chain B:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	25.37Å 41.44Å 65.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	562	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

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	1.23	0/271	2.45	20/416 (4.8%)
1	B	1.27	0/271	2.80	28/416 (6.7%)
All	All	1.25	0/542	2.63	48/832 (5.8%)

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	B	1	0

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	DC	O4'-C1'-N1	19.09	121.36	108.00
1	A	3	DC	O4'-C1'-N1	14.20	117.94	108.00
1	B	15	DC	O4'-C4'-C3'	-13.15	98.11	106.00
1	A	1	DC	P-O3'-C3'	11.70	133.74	119.70
1	B	18	DA	P-O3'-C3'	10.51	132.31	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	23	DC	C3'

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	242	0	136	6	0
1	B	242	0	136	11	0
2	A	34	0	0	2	1
2	B	44	0	0	2	1
All	All	562	0	272	17	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 17 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:23:DC:H2"	1:B:24:DG:C8	2.31	0.65
1:A:8:DT:H2"	1:A:9:DC:C6	2.36	0.61
1:A:4:DA:H1'	2:A:60:HOH:O	2.04	0.56
1:A:9:DC:H2'	1:A:10:DG:C8	2.43	0.54
1:B:22:DG:H2"	1:B:23:DC:C5	2.45	0.52

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	Distance(Å)	Clash(Å)
2:A:79:HOH:O	2:B:47:HOH:O[3_645]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3   RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

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6.3 Carbohydrates ⓘ

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6.4 Ligands ⓘ

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