



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:53 PM GMT

PDB ID : 1D87
Title : CONFORMATIONAL INFLUENCE OF THE RIBOSE 2'-HYDROXYL GROUP: CRYSTAL STRUCTURES OF DNA-RNA CHIMERIC DUPLEXES
Authors : Egli, M.; Usman, N.; Rich, A.
Deposited on : 1992-08-28
Resolution : 2.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

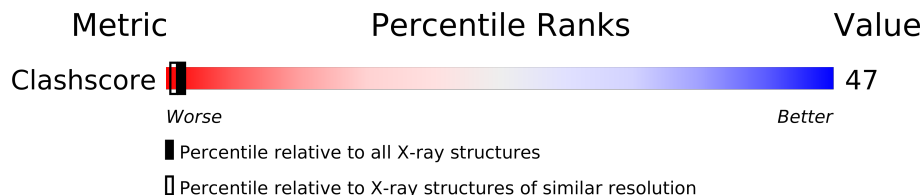
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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	79885	1326 (2.28-2.24)

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	10	
1	B	10	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 516 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 DNA/RNA hybrid called DNA/RNA (5'-R(*GP*)-D(*CP*GP*TP*AP*TP*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			
1	B	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	49	Total	O	0	0
			49	49		

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Note EDS was not executed.

- Chain A:



- Chain B:



4 Data and refinement statistics

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	27.50Å 44.23Å 44.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ (MODIFIED BY G.J.QUIGLEY)	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	516	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	3.47	30/227 (13.2%)	4.74	80/349 (22.9%)
1	B	3.43	29/227 (12.8%)	4.53	72/349 (20.6%)
All	All	3.45	59/454 (13.0%)	4.63	152/698 (21.8%)

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	DA	C2'-C1'	12.67	1.65	1.52
1	B	19	DG	C2-N2	-11.36	1.23	1.34
1	A	9	DG	C2-N2	-11.33	1.23	1.34
1	B	13	DG	C2-N2	-11.03	1.23	1.34
1	B	11	G	C2-N2	-10.81	1.23	1.34

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	DA	P-O3'-C3'	26.43	151.41	119.70
1	B	13	DG	O4'-C4'-C3'	-20.86	93.48	106.00
1	A	9	DG	N3-C2-N2	-15.59	108.98	119.90
1	B	12	DC	N3-C4-C5	-13.86	116.36	121.90
1	B	16	DT	O4'-C4'-C3'	-13.83	97.70	106.00

There are no chirality outliers.

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	203	0	108	11	1
1	B	203	0	108	18	1
2	A	61	0	0	2	5
2	B	49	0	0	2	5
All	All	516	0	216	29	6

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 47.

The worst 5 of 29 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:17:DA:H2'	1:B:18:DC:H5''	1.58	0.86
1:B:20:DC:H6	1:B:20:DC:H5'	1.50	0.77
1:A:8:DC:H2'	1:A:9:DG:C8	2.22	0.74
1:B:11:G:H8	1:B:11:G:HO5'	1.38	0.68
1:B:19:DG:C3'	1:B:20:DC:H5''	2.25	0.66

The worst 5 of 6 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:34:HOH:O	2:B:127:HOH:O[1_655]	1.52	0.68
2:A:35:HOH:O	2:B:117:HOH:O[1_655]	1.65	0.55
2:A:24:HOH:O	2:B:52:HOH:O[1_655]	1.75	0.45
2:A:63:HOH:O	2:B:104:HOH:O[4_565]	1.81	0.39
1:A:4:DT:O2	1:B:11:G:N2[2_664]	1.98	0.22

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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6.5 Other polymers ⓘ

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