



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 09:47 PM GMT

PDB ID : 2X2Q
Title : CRYSTAL STRUCTURE OF AN 'ALL LOCKED' LNA DUPLEX AT 1.9
ANGSTROM RESOLUTION
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C.
Deposited on : 2010-01-15
Resolution : 1.90 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>

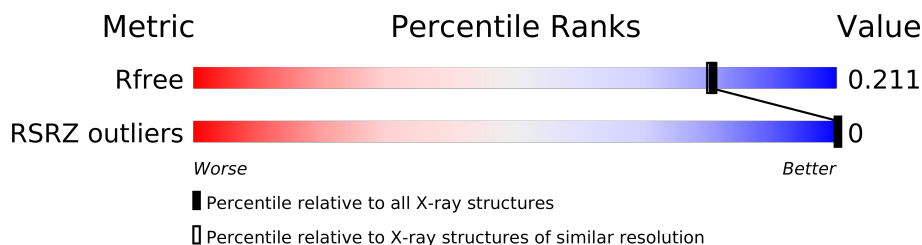
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 1.90 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}	66092	3684 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 MolProbity failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	7	
1	C	7	
2	B	7	
2	D	7	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CAC	A	1008	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 741 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.

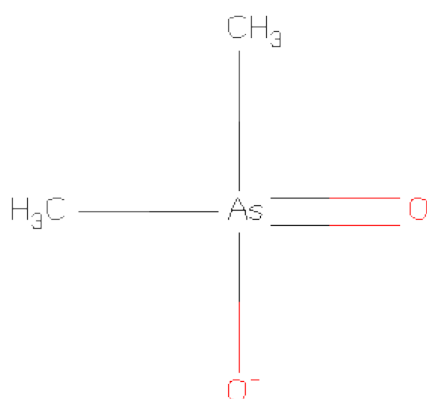
- Molecule 1 is a RNA chain called LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	7	Total 152	C 77	N 22	O 47	P 6	0	0	0
1	C	7	Total 152	C 77	N 22	O 47	P 6	0	0	0

- Molecule 2 is a RNA chain called LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX.

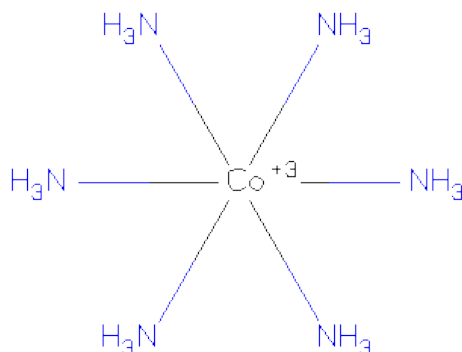
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total 162	C 77	N 32	O 47	P 6	0	0	0
2	D	7	Total 162	C 77	N 32	O 47	P 6	0	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	30	Total	O	0	0
			30	30		
6	C	16	Total	O	0	0
			16	16		
6	D	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		

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 MolProbity failed to run properly.

- Molecule 1: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain A: 

There are no outlier residues recorded for this chain.

- Molecule 1: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 2: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain B: 

There are no outlier residues recorded for this chain.

- Molecule 2: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain D: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.91Å 40.74Å 30.06Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	38.95 – 1.90 36.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.95-1.90) 98.1 (36.10-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.45 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.224 , 0.264 0.230 , 0.211	Depositor DCC
R_{free} test set	341 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 57.9	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 7382 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	741	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.2 Close contacts ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA ⓘ

MolProbity failed to run properly - this section will therefore be empty.

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

MolProbity failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

MolProbity failed to run properly - this section will therefore be empty.

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 ⓘ

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, 95th 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	7/7 (100%)	0.52	0 100 100	24, 31, 41, 41	0
1	C	7/7 (100%)	0.06	0 100 100	25, 32, 41, 41	0
2	B	7/7 (100%)	-0.13	0 100 100	22, 25, 31, 31	0
2	D	7/7 (100%)	-0.48	0 100 100	22, 25, 31, 32	0
All	All	28/28 (100%)	-0.01	0 100 100	22, 30, 41, 41	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LCC	A	66	19/23	0.10	-	32,39,46,46	0
2	LCG	B	7	24/25	0.10	-	28,30,33,35	0
2	TLN	D	3	22/23	0.09	-	20,24,26,27	0
1	LCA	C	70	23/24	0.12	-	23,30,41,45	0
1	LCC	C	66	19/23	0.10	-	32,39,45,46	0
2	LCA	D	5	23/24	0.10	-	27,31,34,35	0
1	LCA	A	70	23/24	0.11	-	22,30,40,45	0
2	LCG	D	4	24/25	0.10	-	25,29,32,32	0
1	LCC	C	67	22/23	0.10	-	31,42,46,48	0
1	TLN	A	68	22/23	0.12	-	35,39,45,47	0
2	LCG	B	1	21/25	0.09	-	19,24,28,33	0
2	LCG	B	2	24/25	0.10	-	19,22,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LCG	D	6	24/25	0.09	-	26,30,32,33	0
2	LCG	B	6	24/25	0.10	-	27,30,31,33	0
2	TLN	B	3	22/23	0.11	-	18,24,25,26	0
1	LCC	A	71	22/23	0.11	-	22,25,32,34	0
1	LCC	C	72	22/23	0.10	-	20,24,27,29	0
2	LCG	B	4	24/25	0.10	-	24,28,31,31	0
1	TLN	C	68	22/23	0.13	-	36,39,45,46	0
1	LCC	C	71	22/23	0.08	-	21,27,32,35	0
1	LCC	A	69	22/23	0.12	-	30,38,42,45	0
2	LCG	D	7	24/25	0.09	-	28,30,33,35	0
2	LCA	B	5	23/24	0.10	-	25,31,34,35	0
1	LCC	A	67	22/23	0.12	-	32,42,45,48	0
2	LCG	D	1	21/25	0.10	-	19,24,28,32	0
1	LCC	A	72	22/23	0.10	-	19,23,27,28	0
2	LCG	D	2	24/25	0.09	-	19,21,24,26	0
1	LCC	C	69	22/23	0.12	-	31,38,44,46	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NCO	B	1008	7/7	0.14	-	26,27,29,30	0
5	MG	C	1008	1/1	0.11	-	18,18,18,18	1
3	CAC	A	1008	5/5	0.15	-	84,86,86,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.