Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 06:33 AM EST

PDB ID	:	1NUJ
Title	:	THE LEADZYME STRUCTURE BOUND TO MG(H20)6(II) AT 1.8 A RESOLUTION
Authors	:	Wedekind, J.E.; Mckay, D.B.
Deposited on	:	2003-01-31
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

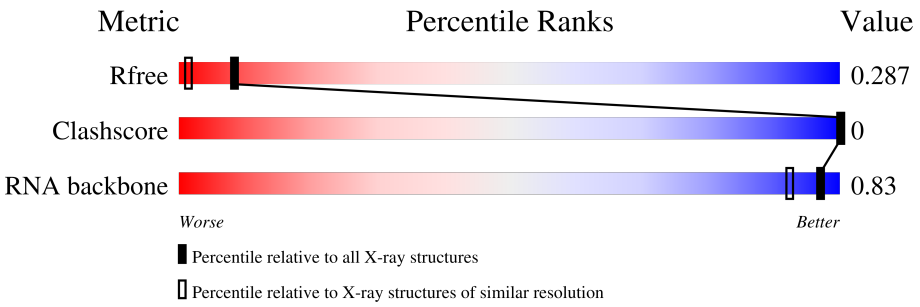
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
RNA backbone	3102	1060 (2.40-1.20)

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%

Mol	Chain	Length	Quality of chain
1	A	13	85% 15%
1	C	13	85% 15%
1	E	13	85% 8% 8%
1	G	13	85% 8% 8%
2	B	11	91% 9%
2	D	11	91% 9%
2	F	11	91% 9%
2	H	11	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2498 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 5'-R(*CP*GP*GP*AP*CP*CP*GP*AP*GP*CP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	13	290	131	60	87	12	0	1	0
1	C	13	278	125	55	86	12	1	0	0
1	E	13	278	125	55	86	12	0	0	0
1	G	13	290	131	60	87	12	0	1	0

- Molecule 2 is a RNA chain called 5'-R(*GP*CP*UP*GP*GP*GP*AP*GP*UP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	234	105	43	76	10	0	0	0
2	D	11	234	105	43	76	10	0	0	0
2	F	11	234	105	43	76	10	0	0	0
2	H	11	234	105	43	76	10	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	1	1	1	0	0
3	C	2	2	2	0	0
3	E	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	G	2	2	2	0	0
			Total	Mg		
3	H	1	1	1	0	0

- Molecule 4 is water.

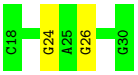
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	50	50	50	0	0
			Total	O		
4	B	46	46	46	0	0
			Total	O		
4	C	62	62	62	0	0
			Total	O		
4	D	47	47	47	0	0
			Total	O		
4	E	62	62	62	0	0
			Total	O		
4	F	53	53	53	0	0
			Total	O		
4	G	56	56	56	0	0
			Total	O		
4	H	40	40	40	0	0

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. 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.

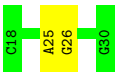
- Molecule 1: 5'-R(*CP*GP*GP*AP*CP*CP*GP*AP*GP*CP*CP*AP*G)-3'

Chain A:



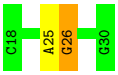
- Molecule 1: 5'-R(*CP*GP*GP*AP*CP*CP*GP*AP*GP*CP*CP*AP*G)-3'

Chain C:



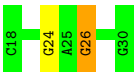
- Molecule 1: 5'-R(*CP*GP*GP*AP*CP*CP*GP*AP*GP*CP*CP*AP*G)-3'

Chain E:



- Molecule 1: 5'-R(*CP*GP*GP*AP*CP*CP*GP*AP*GP*CP*CP*AP*G)-3'

Chain G:



- Molecule 2: 5'-R(*GP*CP*UP*GP*GP*GP*AP*GP*UP*CP*C)-3'

Chain B:

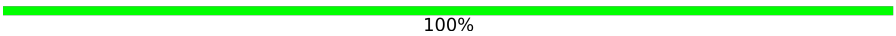
- Molecule 2: 5'-R(*GP*CP*UP*GP*GP*GP*AP*GP*UP*CP*C)-3'

Chain D:

• Molecule 2: 5'-R(*GP*CP*UP*GP*GP*GP*AP*GP*UP*CP*C)-3'

Chain F:

• Molecule 2: 5'-R(*GP*CP*UP*GP*GP*GP*AP*GP*UP*CP*C)-3'

Chain H: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	60.10Å 60.10Å 133.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.31 – 1.80 29.31 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.31-1.80) 94.2 (29.31-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.224 0.271 , 0.287	Depositor DCC
R_{free} test set	2207 reflections (9.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2498	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 25.46 % 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 3.1570e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.54	0/337	0.82	0/525
1	C	0.65	0/311	0.86	0/484
1	E	0.67	0/311	0.84	1/484 (0.2%)
1	G	0.55	0/337	0.84	2/525 (0.4%)
2	B	0.58	0/261	0.69	0/406
2	D	0.72	0/261	0.72	0/406
2	F	0.65	0/261	0.69	0/406
2	H	0.61	0/261	0.69	0/406
All	All	0.62	0/2340	0.78	3/3642 (0.1%)

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	0	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	11

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	26[A]	G	C5'-C4'-C3'	-5.58	107.08	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	26[B]	G	C5'-C4'-C3'	-5.58	107.08	116.00
1	E	26	G	O4'-C1'-N9	5.37	112.49	108.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26[A]	G	Sidechain
1	A	26[B]	G	Sidechain
2	B	47	U	Sidechain
1	C	25	A	Sidechain
1	C	26	G	Sidechain
2	D	49	C	Sidechain
1	E	25	A	Sidechain
1	E	26	G	Sidechain
2	F	49	C	Sidechain
1	G	26[A]	G	Sidechain
1	G	26[B]	G	Sidechain

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	290	0	144	0	0
1	C	278	0	145	0	0
1	E	278	0	145	0	0
1	G	290	0	144	0	0
2	B	234	0	121	0	0
2	D	234	0	121	0	0
2	F	234	0	121	0	0
2	H	234	0	121	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	0	0	0
4	B	46	0	0	0	0
4	C	62	0	0	0	0
4	D	47	0	0	0	0
4	E	62	0	0	0	0
4	F	53	0	0	0	0
4	G	56	0	0	0	0
4	H	40	0	0	0	0
All	All	2498	0	1062	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	11/13 (84%)	1 (9%)	0
1	C	12/13 (92%)	0	0
1	E	12/13 (92%)	0	0
1	G	11/13 (84%)	1 (9%)	0
2	B	10/11 (90%)	0	0
2	D	10/11 (90%)	0	0
2	F	10/11 (90%)	0	0
2	H	10/11 (90%)	0	0
All	All	86/96 (89%)	2 (2%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	24	G
1	G	24	G

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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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 (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.