WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 06:08 PM EDT

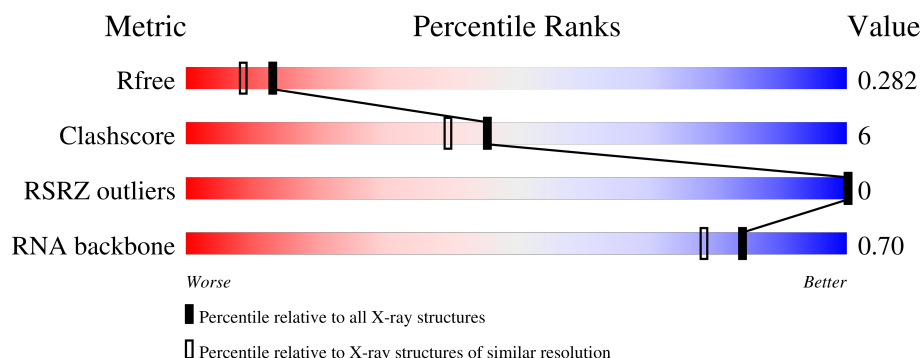|		
PDB ID	:	1ZX7
Title	:	Molecular Recognition of RNA by Neomycin and a Restricted Neomycin Derivative
Authors	:	Zhao, Q.; Zhao, F.; Blount, K.F.; Han, Q.; Tor, Y.; Hermann, T.
Deposited on	:	2005-06-07
Resolution	:	2.15 Å(reported)

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 2.15 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.
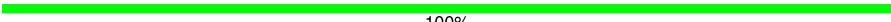
Metric	Percentile Ranks	Value
Rfree		0.282
Clashscore		6
RSRZ outliers		0
RNA backbone		0.70

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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	15	53% / 40% / 7%
1	C	15	73% / 20% / 7%
1	E	15	53% / 27% / 20%
1	G	15	53% / 33% / 13%
2	B	14	71% / 29%
2	D	14	50% / 50%

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Mol	Chain	Length	Quality of chain
2	F	14	100%
2	H	14	64% 36%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2548 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(*GP*UP*GP*GP*UP*GP*AP*AP*GP*UP*CP*GP*CP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			325	145	62	104	14			
1	C	15	Total	C	N	O	P	0	0	0
			325	145	62	104	14			
1	E	15	Total	C	N	O	P	0	0	0
			325	145	62	104	14			
1	G	15	Total	C	N	O	P	0	0	0
			325	145	62	104	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			289	131	51	94	13			
2	D	14	Total	C	N	O	P	0	0	0
			289	131	51	94	13			
2	F	14	Total	C	N	O	P	0	0	0
			289	131	51	94	13			
2	H	14	Total	C	N	O	P	0	0	0
			289	131	51	94	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	8	Total	O	0	0
			8	8		
3	C	19	Total	O	0	0
			19	19		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	5	Total 5	O 5	0	0
3	E	11	Total 11	O 11	0	0
3	F	10	Total 10	O 10	0	0
3	G	12	Total 12	O 12	0	0
3	H	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

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 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.

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

Chain A:

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

Chain C:

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

Chain E:

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

Chain G:

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

Chain B:

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

Chain D:

C21 U25 C26 A27 C30 C31 A32 C33 C34
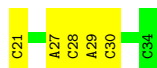
• Molecule 2: 5'-R(*CP*GP*CP*GP*UP*CP*AP*CP*AP*CP*CP*AP*CP*C)-3'

Chain F: 100%

There are no outlier residues recorded for this chain.

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

Chain H: 64% 36%

C21 A27 C28 A29 C30 C34

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	32.65Å 153.20Å 32.74Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.15 27.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.3 (8.00-2.15) 88.8 (27.56-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.292 0.263 , 0.282	Depositor DCC
R_{free} test set	1625 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 15.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.458 for l,k,-h 0.478 for h,-k,-l 0.466 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2548	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 28.13 % 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 1.9450e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

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	0.35	0/364	0.66	0/568
1	C	0.47	0/364	0.72	0/568
1	E	0.47	0/364	0.76	0/568
1	G	0.41	0/364	0.71	0/568
2	B	0.41	0/321	0.67	0/497
2	D	0.36	0/321	0.71	0/497
2	F	0.37	0/321	0.62	0/497
2	H	0.38	0/321	0.67	0/497
All	All	0.41	0/2740	0.69	0/4260

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	C	0	1
1	E	0	1
1	G	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	U	Sidechain
2	D	25	U	Sidechain
1	E	11	U	Sidechain
1	G	11	U	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	325	0	164	5	1
1	C	325	0	164	1	0
1	E	325	0	164	4	0
1	G	325	0	164	7	0
2	B	289	0	155	2	0
2	D	289	0	155	4	1
2	F	289	0	155	0	0
2	H	289	0	155	3	0
3	A	18	0	0	0	0
3	B	8	0	0	0	0
3	C	19	0	0	0	0
3	D	5	0	0	0	0
3	E	11	0	0	0	0
3	F	10	0	0	0	0
3	G	12	0	0	0	0
3	H	9	0	0	0	0
All	All	2548	0	1276	24	1

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 6.

The worst 5 of 24 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)
1:G:15:G:H1	2:H:21:C:H42	1.46	0.64
1:A:8:A:H2'	1:A:9:A:O4'	1.98	0.63
1:G:15:G:H2'	1:G:16:G:H8	1.67	0.58
1:E:11:U:H2'	1:E:12:C:O4'	2.09	0.52
1:E:8:A:O2'	1:E:9:A:H5'	2.11	0.51

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:A:O2'	2:D:32:A:O4'[1_554]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	14/15 (93%)	2 (14%)	0
1	C	14/15 (93%)	2 (14%)	1 (7%)
1	E	14/15 (93%)	1 (7%)	1 (7%)
1	G	14/15 (93%)	1 (7%)	1 (7%)
2	B	13/14 (92%)	0	0
2	D	13/14 (92%)	0	0
2	F	13/14 (92%)	0	0
2	H	13/14 (92%)	0	0
All	All	108/116 (93%)	6 (5%)	3 (2%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	10	G
1	C	12	C
1	C	13	G
1	E	13	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	12	C
1	E	12	C
1	G	7	G

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 monosaccharides 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 ⓘ

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(Å²)	Q<0.9
1	A	15/15 (100%)	-0.12	0	100	100	21, 28, 37, 44	0
1	C	15/15 (100%)	-0.17	0	100	100	22, 25, 37, 37	0
1	E	15/15 (100%)	-0.24	0	100	100	23, 26, 37, 44	0
1	G	15/15 (100%)	-0.13	0	100	100	23, 26, 35, 43	0
2	B	14/14 (100%)	-0.21	0	100	100	20, 27, 33, 35	0
2	D	14/14 (100%)	-0.09	0	100	100	18, 32, 43, 45	0
2	F	14/14 (100%)	-0.05	0	100	100	19, 27, 36, 38	0
2	H	14/14 (100%)	-0.15	0	100	100	20, 29, 39, 44	0
All	All	116/116 (100%)	-0.15	0	100	100	18, 27, 39, 45	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.